METHODS OF MODERN MATHEMATICAL PHYSICS

II: FOURIER ANALYSIS, SELF-ADJOINTNESS

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To our parents
Helen and Gerald Reed
Minnie and Hy Simon

Preface

This volume continues our series of texts devoted to functional analysis methods in mathematical physics. In Volume I we announced a table of contents for Volume II. However, in the preparation of the material it became clear that we would be unable to treat the subject matter in sufficient depth in one volume. Thus, the volume contains Chapters IX and X; we expect that a third volume will appear in the near future containing the rest of the material announced as "Analysis of Operators." We hope to continue this series with an additional volume on algebraic methods.

It gives us pleasure to thank many individuals:

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MIKE REED
BARRY SIMON

June 1975

Introduction

A functional analyst is an analyst, first and foremost, and not a degenerate species of topologist.
E. Hille

Most texts in functional analysis suffer from a serious defect that is shared to an extent by Volume I of Methods of Modern Mathematical Physics. Namely, the subject is presented as an abstract, elegant corpus generally divorced from applications. Consequently, the students who learn from these texts are ignorant of the fact that almost all deep ideas in functional analysis have their *immediate* roots in "applications," either to classical areas of analysis such as harmonic analysis or partial differential equations, or to another science, primarily physics. For example, it was classical electromagnetic potential theory that motivated Fredholm's work on integral equations and thereby the work of Hilbert, Schmidt, Weyl, and Riesz on the abstractions of Hilbert space and compact operator theory. And it was the impetus of quantum mechanics that led von Neumann to his development of unbounded operators and later to his work on operator algebras.

More deleterious than historical ignorance is the fact that students are too often misled into believing that the most profitable directions for research in functional analysis are the abstract ones. In our opinion, exactly the opposite is true. We do not mean to imply that abstraction has no role to play. Indeed, it has the critical role of taking an idea from a concrete situation and, by eliminating the extraneous notions, making the idea more easily understood as well as applicable to a broader range of

situations. But it is the study of specific applications and the consequent generalizations that have been the more important, rather than the consideration of abstract questions about abstract objects for their own sake.

This volume contains a mixture of abstract results and applications, while the next contains mainly applications. The intention is to offer the readers of the whole series a properly balanced view.

We hope that this volume will serve several purposes: to provide an introduction for graduate students not previously acquainted with the material, to serve as a reference for mathematical physicists already working in the field, and to provide an introduction to various advanced topics which are difficult to understand in the literature. Not all the techniques and applications are treated in the same depth. In general, we give a very thorough discussion of the mathematical techniques and applications in quantum mechanics, but provide only an introduction to the problems arising in quantum field theory, classical mechanics, and partial differential equations. Finally, some of the material developed in this volume will not find application until Volume III. For all these reasons, this volume contains a great variety of subject matter. To help the reader select which material is important for him, we have provided a "Reader's Guide" at the end of each chapter.

As in Volume I, each chapter contains a section of notes. The notes give references to the literature and sometimes extend the discussion in the text. Historical comments are always limited by the knowledge and prejudices of authors, but in mathematics that arises directly from applications, the problem of assigning credit is especially difficult. Typically, the history is in two stages: first a specific method (typically difficult, computational, and sometimes nonrigorous) is developed to handle a small class of problems. Later it is recognized that the method contains ideas which can be used to treat other problems, so the study of the method itself becomes important. The ideas are then abstracted, studied on the abstract level, and the techniques systematized. With the newly developed machinery the original problem becomes an easy special case. In such a situation, it is often not completely clear how many of the mathematical ideas were already contained in the original work. Further, how one assigns credit may depend on whether one first learned the technique in the old computational way or in the new easier but more abstract way. In such situations, we hope that the reader will treat the notes as an introduction to the literature and not as a judgment of the historical value of the contributions in the papers cited.

Each chapter ends with a set of problems. As in Volume I, parts of proofs are occasionally left to the problems to encourage the reader to

participate in the development of the mathematics. Problems that fill gaps in the text are marked with a dagger. Difficult problems are marked with an asterisk. We strongly urge students to work the problems since that is the best way to learn mathematics.

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IX: The Fourier Transform

We have therefore the equation of condition

$$F(x) = \int dq\, Q \cos qx$$

If we substituted for Q any function of q, and conducted the integration from $q = 0$ to $q = \infty$, we should find a function of x: it is required to solve the inverse problem, that is to say, to ascertain what function of q, after being substituted for Q, gives as a result the function $F(x)$, a remarkable problem whose solution demands attentive examination. *Joseph Fourier*

IX.1 The Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$, convolutions

The Fourier transform is an important tool of both classical and modern analysis. We begin by defining it, and the inverse transform, on $\mathscr{S}(\mathbb{R}^n)$, the Schwartz space of C^∞ functions of rapid decrease.

Definition Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. The **Fourier transform** of f is the function $\hat{f}$ given by

$$\hat{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\mathbf{x}\cdot\lambda} f(\mathbf{x})\, d\mathbf{x}$$

where $\mathbf{x} \cdot \lambda = \sum_{i=1}^n x_i \lambda_i$. The **inverse Fourier transform** of f, denoted by $\check{f}$, is the function

$$\check{f}(\lambda) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{i\mathbf{x}\cdot\lambda} f(\mathbf{x})\, d\mathbf{x}$$

We will occasionally write $\hat{f} = \mathscr{F}f$.

Since every function in Schwartz space is in $L^1(\mathbb{R}^n)$, the above integrals make sense. Many authors begin by discussing the Fourier transform on $L^1(\mathbb{R}^n)$. We start with Schwartz space for two reasons: First, the Fourier transform is a one-to-one map of Schwartz space onto itself (Theorem IX.1). This makes it particularly easy to talk about the inverse Fourier transform, which of course turns out to be the inverse map. That is, on Schwartz space, it is possible to deal with the transform and the inverse transform on an equal footing. Though this is also true for the Fourier transform on $L^2(\mathbb{R}^n)$ (see Theorem IX.6), it is not possible to define the Fourier transform on $L^2(\mathbb{R}^n)$ directly by the integral formula since $L^2(\mathbb{R}^n)$ functions may not be in $L^1(\mathbb{R}^n)$; a limiting procedure must be used. Secondly, once we know that the Fourier transform is a one-to-one, bounded map of $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$, we can easily extend it to $\mathscr{S}'(\mathbb{R}^n)$. It is this extension that is fundamental to the applications in Sections 5, 6, and 8.

We will use the standard multi-index notation. A multi-index

$$\alpha = \langle \alpha_1, \ldots, \alpha_n \rangle$$

is an n-tuple of nonnegative integers. The collection of all multi-indices will be denoted by I_+^n. The symbols $|\alpha|$, x^α, D^α, and x^2 are defined as follows:

$$|\alpha| = \sum_{i=1}^n \alpha_i$$

$$x^\alpha = x_1^{\alpha_1} x_2^{\alpha_2} \cdots x_n^{\alpha_n}$$

$$D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1}\, \partial x_2^{\alpha_2} \cdots \partial x_n^{\alpha_n}}$$

$$x^2 = \sum_{i=1}^n x_i^2$$

In preparation for the proof that $\hat{}$ and $\check{}$ are inverses, we prove:

Lemma The maps $\hat{}$ and $\check{}$ are continuous linear transformations of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if α and β are multi-indices, then

$$((i\lambda)^\alpha D^\beta \hat{f})(\lambda) = \widehat{D^\alpha((-ix)^\beta f(x))} \tag{IX.1}$$

Proof The map $\hat{}$ is clearly linear. Since

$$\begin{aligned}(\lambda^\alpha D^\beta \hat{f})(\lambda) &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \lambda^\alpha (-ix)^\beta e^{-i\lambda\cdot x} f(x)\, dx \\ &= \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{1}{(-i)^\alpha} (D_x^\alpha e^{-i\lambda\cdot x})(-ix)^\beta f(x)\, dx \\ &= \frac{(-i)^\alpha}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} e^{-i\lambda\cdot x} D_x^\alpha((-ix)^\beta f(x))\, dx\end{aligned}$$

We conclude that

$$\|\hat{f}\|_{\alpha,\beta} = \sup_\lambda |\lambda^\alpha (D^\beta \hat{f})(\lambda)| \le \frac{1}{(2\pi)^{n/2}} \int |D_x^\alpha (x^\beta f)|\, dx < \infty$$

so $\hat{}$ takes $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, and we have also proven (IX.1). Furthermore, if k is large enough, $\int (1+x^2)^{-k}\, dx < \infty$ so that

$$\begin{aligned}\|\hat{f}\|_{\alpha,\beta} &\le \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \frac{(1+x^2)^{-k}}{(1+x^2)^{-k}} |D_x^\alpha(-ix)^\beta f(x)|\, dx \\ &\le \frac{1}{(2\pi)^{n/2}} \left(\int (1+x^2)^{-k}\, dx \right) \sup_x \{(1+x^2)^{+k} |D_x^\alpha(-ix)^\beta f(x)|\}\end{aligned}$$

Using Leibnitz's rule we easily conclude that there exist multi-indices α_j, β_j and constants c_j so that

$$\|\hat{f}\|_{\alpha,\beta} \le \sum_{j=1}^M c_j \|f\|_{\alpha_j,\beta_j}$$

Thus, $\hat{}$ is bounded and by Theorem V.4 is therefore continuous. The proof for $\check{}$ is the same. ∎

We are now ready to prove the Fourier inversion theorem. The proof we give uses the original idea of Fourier.

Theorem IX.1 (Fourier inversion theorem) The Fourier transform is a linear bicontinuous bijection from $\mathscr{S}(\mathbb{R}^n)$ onto $\mathscr{S}(\mathbb{R}^n)$. Its inverse map is the inverse Fourier transform, i.e., $\check{\hat{f}} = f = \hat{\check{f}}$.

Proof We will prove that $\check{\hat{f}} = f$. The proof that $\hat{\check{f}} = f$ is similar. $\hat{\check{f}} = f$ implies that $\hat{}$ is surjective and $\check{\hat{f}} = f$ implies that $\hat{}$ is injective. Since $\hat{}$ and $\check{}$ are continuous maps of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$, it is sufficient to prove that $\check{\hat{f}} = f$ for f contained in the dense set $C_0^\infty(\mathbb{R}^n)$. Let C_ε be the cube of volume $(2/\varepsilon)^n$ centered at the origin in $\mathbb{R}^n$. Choose ε small enough so that the support of f is contained in C_ε. Let

$$K_\varepsilon = \{\mathbf{k} \in \mathbb{R} \,|\, \text{each } k_i/\pi\varepsilon \text{ is an integer}\}$$

Then

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}, f)(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}$$

is just the Fourier series of f which converges uniformly in C_ε to f since f is continuously differentiable (Theorem II.8). Thus

$$f(x) = \sum_{k \in K_\varepsilon} \frac{\hat{f}(k) e^{ik\cdot x}}{(2\pi)^{n/2}} (\pi\varepsilon)^n \tag{IX.2}$$

Since $\mathbb{R}^n$ is the disjoint union of the cubes of volume $(\pi\varepsilon)^n$ centered about the points in K_ε, the right-hand side of (IX.2) is just a Riemann sum for the integral of the function $\hat{f}(k)e^{ik\cdot x}/(2\pi)^{n/2}$. By the lemma, $\hat{f}(k)e^{ik\cdot x} \in \mathscr{S}(\mathbb{R}^n)$, so the Riemann sums converge to the integral. Thus $\check{\hat{f}} = f$. ∎

Corollary Suppose $f \in \mathscr{S}(\mathbb{R}^n)$. Then

$$\int_{\mathbb{R}^n} |f(x)|^2\, dx = \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk$$

Proof This is really a corollary of the proof rather than the statement of Theorem IX.1. If f has compact support, then for ε small enough,

$$f(x) = \sum_{k \in K_\varepsilon} ((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))(\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}$$

Since $\{(\frac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x}\}_{k\in K_\varepsilon}$ is an orthonormal basis for $L^2(C_\varepsilon)$,

$$\begin{aligned}\int_{\mathbb{R}^n} |f(x)|^2\, dx &= \int_{C_\varepsilon} |f(x)|^2\, dx \\ &= \sum_{k\in K_\varepsilon} |((\tfrac{1}{2}\varepsilon)^{n/2} e^{ik\cdot x},\ f(x))|^2 \\ &= \sum_{k\in K_\varepsilon} |\hat{f}(k)|^2 (\pi\varepsilon)^n \\ &\xrightarrow[\varepsilon\to 0]{} \int_{\mathbb{R}^n} |\hat{f}(k)|^2\, dk\end{aligned}$$

This proves the corollary for $f \in C_0^\infty$. Since $\hat{}$ and $\|\cdot\|_2$ are continuous on $\mathscr{S}$ and C_0^∞ is dense, the result holds for all of $\mathscr{S}$. ∎

Example 1 We compute the Fourier transform of $f(x) = e^{-\alpha x^2/2} \in \mathscr{S}(\mathbb{R})$ where $\alpha > 0$.

$$\begin{aligned}\hat{f}(\lambda) &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-\alpha x^2/2} e^{-i\lambda\cdot x}\, dx \\ &= \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \sqrt{\frac{2}{\alpha}} \exp\left(-t^2 - it\lambda\sqrt{\frac{2}{\alpha}}\right) dt \\ &= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} \exp -\left(t + i\frac{\lambda}{\sqrt{2\alpha}}\right)^2 dt \\ &= \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha\pi}} \int_{\mathbb{R}} e^{-t^2}\, dt = \frac{e^{-\lambda^2/2\alpha}}{\sqrt{\alpha}}\end{aligned}$$

The next to last step follows from the Cauchy integral formula and the exponential decrease of e^{-z^2} along lines parallel to the x axis.

We now define the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$.

Definition Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Then the Fourier transform of T, denoted by $\hat{T}$, is the tempered distribution defined by $\hat{T}(\varphi) = T(\hat{\varphi})$.

Suppose that $h,\ \varphi \in \mathscr{S}(\mathbb{R}^n)$, then by the polarization identity and the corollary to Theorem IX.1 we have $(h, \varphi) = (\hat{h}, \hat{\varphi})$. Substituting $\check{\tilde{g}} = \check{\bar{g}}$ for h, we obtain

$$T_{\hat{g}}(\varphi) = \int \hat{g}(x)\varphi(x)\, dx = \int g(x)\hat{\varphi}(x)\, dx = T_g(\hat{\varphi}) = \hat{T}_g(\varphi)$$

where $T_{\hat{g}}$ and T_g are the distributions corresponding to the functions $\hat{g}$ and g respectively. This shows that the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ extends the transform we previously defined on $\mathscr{S}(\mathbb{R}^n)$.

Theorem IX.2 The Fourier transform is a one-to-one linear bijection from $\mathscr{S}'(\mathbb{R}^n)$ to $\mathscr{S}'(\mathbb{R}^n)$ which is the unique weakly continuous extension of the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$.

Proof If $\varphi_n \xrightarrow{\mathscr{S}} \varphi$, then by Theorem IX.1, $\hat{\varphi}_n \xrightarrow{\mathscr{S}} \hat{\varphi}$, so $T(\hat{\varphi}_n) \to T(\hat{\varphi})$ for each T in $\mathscr{S}'(\mathbb{R}^n)$. Thus $\hat{T}(\varphi_n) \to \hat{T}(\varphi)$, which shows that $\hat{T}$ is a continuous linear functional on $\mathscr{S}(\mathbb{R}^n)$. Furthermore, if $T_n \xrightarrow{w} T$, then $\hat{T}_n \xrightarrow{w} \hat{T}$ because $T_n(\hat{\varphi}) \to T(\hat{\varphi})$ implies $\hat{T}_n(\varphi) \to \hat{T}(\varphi)$. Thus $T \mapsto \hat{T}$ is weakly continuous.

The remaining properties of $\hat{}$ follow immediately from the corresponding statements on $\mathscr{S}(\mathbb{R}^n)$ (see Problem 19 in Chapter V). ∎

Example 2 We compute the Fourier transform of the derivative of the delta function at $b \in \mathbb{R}$:

$$\begin{aligned}\hat{\delta}_b'(\varphi) &= \delta_b'(\hat{\varphi}) \\ &= \delta_b\left(-\frac{d}{d\lambda}\hat{\varphi}(\lambda)\right) \\ &= \delta_b\left(\frac{-1}{(2\pi)^{1/2}} \int e^{-i\lambda x}(-ix)\varphi(x)\, dx\right) \\ &= \int \left(\frac{ixe^{-ibx}}{\sqrt{2\pi}}\right)\varphi(x)\, dx\end{aligned}$$

So, the Fourier transform of δ_b' is the function $ixe^{-ibx}/\sqrt{2\pi}$.

* * *

We now introduce a new operation on functions.

Definitions Suppose that $f, g \in \mathscr{S}(\mathbb{R}^n)$. Then the **convolution** of f and g, denoted by $f * g$, is the function

$$(f * g)(y) = \int_{\mathbb{R}^n} f(y - x)g(x)\, dx$$

The convolution arises in many circumstances (we have already used it in discussing closed operators in Section VIII.1). In Section 4 we use interpolation theorems to prove L^p estimates on the convolution $f * g$ in terms of f and g. In this section we concentrate on the properties of the convolution as a map from $\mathscr{S}(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to $\mathscr{S}(\mathbb{R}^n)$. Using these properties we show that the convolution can be extended to a map from $\mathscr{S}'(\mathbb{R}^n) \times \mathscr{S}(\mathbb{R}^n)$ to O_M^n, the polynomially bounded C^∞ functions. Convolutions frequently occur when one uses the Fourier transform because the Fourier transform takes products into convolutions (Theorem IX.3b and Theorem IX.4c).

Theorem IX.3

(a) For each $f \in \mathscr{S}(\mathbb{R}^n)$, $g \to f * g$ is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

(b) $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$ and $\widehat{f * g} = (2\pi)^{n/2}\hat{f}\hat{g}$.

(c) For f, g, h, in $\mathscr{S}(\mathbb{R}^n)$, $f * g = g * f$ and $f * (g * h) = (f * g) * h$.

Proof From the polarization identity and the corollary to Theorem IX.1 we find that $(\varphi, \psi) = (\hat{\varphi}, \hat{\psi})$ for $\varphi, \psi \in \mathscr{S}(\mathbb{R}^n)$. Letting $y \in \mathbb{R}^n$ be fixed, we apply this identity to $e^{iy \cdot x}\check{f}(x)$ and g obtaining $(e^{iy \cdot x}\check{f}, g) = (\widehat{e^{iy \cdot x}\check{f}}, \hat{g})$. But

$$(e^{iy \cdot x}\check{f}, g) = \int_{\mathbb{R}^n} e^{-iy \cdot x} f(x)g(x)\, dx$$

and

$$(\widehat{e^{iy \cdot x}\check{f}}, \hat{g}) = \int_{\mathbb{R}^n} \left(\overline{(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda \cdot x + iy \cdot x} \overline{f(x)}\, dx} \right) \hat{g}(\lambda)\, d\lambda$$

$$= \int_{\mathbb{R}^n} \hat{f}(y - \lambda)\hat{g}(\lambda)\, d\lambda$$

which proves that $\widehat{fg} = (2\pi)^{-n/2}\hat{f} * \hat{g}$. Using the inverse Fourier transform this formula may be stated as

$$(2\pi)^{n/2}\widehat{\check{f}\check{g}} = f * g$$

This shows that convolution is the composition of the inverse Fourier transform, multiplication by $(2\pi)^{n/2}\check{f}$, and the Fourier transform. It follows that convolution is continuous.

The statements in (c) follow trivially from (b). ∎

In order to extend the map $C_f : g \to f * g$ to $\mathscr{S}'$, we look for a continuous map $\tilde{C}_f : \mathscr{S} \to \mathscr{S}$ so that $\tilde{C}_f' \restriction \mathscr{S} = C_f$. We then define $\tilde{C}_f'$ to be convolution on $\mathscr{S}'$.

Definition Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$, $T \in \mathscr{S}'(\mathbb{R}^n)$ and let $\tilde{f}(x)$ denote the function, $f(-x)$. Then, the **convolution** of T and f, denoted $T * f$, is the distribution in $\mathscr{S}'(\mathbb{R}^n)$ given by

$$(T * f)(\varphi) = T(\tilde{f} * \varphi)$$

for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$.

The fact that $g \to \tilde{f} * g$ is a continuous transformation guarantees that $T * f \in \mathscr{S}'(\mathbb{R}^n)$. The following theorem summarizes the properties of this extended convolution.

Let f_y denote the function $f_y(x) = f(x - y)$ and $\tilde{f}_y$ the function $f(y - x)$. When f is given by a large expression $(\cdots)$, we will sometimes write $(\cdots)^{\sim}$ rather than $(\cdot\tilde{\cdot}\cdot)$.

Theorem IX.4 For each $f \in \mathscr{S}(\mathbb{R}^n)$ the map $T \to T * f$ is a weakly continuous map of $\mathscr{S}'(\mathbb{R}^n)$ into $\mathscr{S}'(\mathbb{R}^n)$ which extends the convolution on $\mathscr{S}(\mathbb{R}^n)$. Furthermore,

(a) $T * f$ is a polynomially bounded C^∞ function, i.e. $T * f \in O_M^n$. In fact, $(T * f)(y) = T(\tilde{f}_y)$ and

$$D^\beta(T * f) = (D^\beta T) * f = T * D^\beta f \tag{IX.3}$$

(b) $(T * f) * g = T * (f * g)$

(c) $\widehat{T * f} = (2\pi)^{n/2}\hat{f}\hat{T}$

Proof Since $T \to T * f$ is defined as the adjoint of a bounded map from $\mathscr{S}$ to $\mathscr{S}$, it is automatically weakly continuous. The fact that it extends the convolution on $\mathscr{S}$ is just a change of variables. The statements (IX.3), (b), and (c), all follow immediately from the corresponding statements for $T \in \mathscr{S}$ and the facts that $\mathscr{S}$ is weakly dense in $\mathscr{S}'$ and that $\mathscr{F}$, D^β, multiplication by $\hat{f}$, and convolution are all weakly continuous on $\mathscr{S}'$.

It remains to prove the first part of (a). Since $T \in \mathscr{S}'(\mathbb{R}^n)$, it follows from the regularity theorem (Theorem V.10) that there is a bounded continuous function h, a positive integer r, and a multi-index β so that

$$T(\tilde{f}_y) = \int_{\mathbb{R}^n} h(x)(1 + x^2)^r (D^\beta f)(y - x)\, dx$$

Since $D^\beta f \in \mathscr{S}$, $T(\tilde{f}_y)$ is an infinitely differentiable function of y. The change of variables $\tau = y - x$ shows that

$$|T(\tilde{f}_y)| \leq \|h\|_\infty \int_{\mathbb{R}^n} (1 + x^2)^r |(D^\beta f)(y - x)|\, dx$$

$$= \|h\|_\infty \int_{\mathbb{R}^n} (1 + (y - \tau)^2)^r |D^\beta f(\tau)|\, d\tau$$

from which it follows easily that $y \mapsto T(\tilde{f}_y)$ is polynomially bounded. A similar proof works for the derivatives of $y \mapsto T(\tilde{f}_y)$. Thus $T(\tilde{f}_y) \in O_M^n$.

Suppose that a distribution $S \in \mathscr{S}'(\mathbb{R}^n)$ is given by a polynomially bounded continuous function s. Then, using Fubini's theorem we find that for $\varphi \in \mathscr{S}(\mathbb{R}^n)$

$$\begin{aligned}(S * f)(\varphi) &\equiv S(\tilde{f} * \varphi) \\ &= \int s(x)\left(\int \tilde{f}(x - y)\varphi(y)\, dy\right) dx \\ &= \int \left(\int s(x)\tilde{f}_y(x)\, dx\right)\varphi(y)\, dy \\ &= (S(\tilde{f}_y))(\varphi)\end{aligned}$$

so $S * f = S(\tilde{f}_y)$. By the regularity theorem $T = D^\alpha S$ for some such S. Thus by (IX.3)

$$\begin{aligned}T * f = (D^\alpha S) * f &= S * D^\alpha f \\ &= S((D^\alpha f)^\sim_y) \\ &= (-1)^{|\alpha|} S(D^\alpha(\tilde{f}_y)) \\ &= D^\alpha S(\tilde{f}_y) \\ &= T(\tilde{f}_y)\end{aligned}$$

This completes the proof. ∎

Theorem IX.5 Let $T \in \mathscr{S}'(\mathbb{R}^n)$ and $f \in \mathscr{S}(\mathbb{R}^n)$. Then $\widehat{fT} \in O_M^n$ and $\widehat{fT}(k) = (2\pi)^{-n/2} T(fe^{-ik\cdot x})$. In particular, if T has compact support and $\psi \in \mathscr{S}(\mathbb{R}^n)$ is identically one on a neighborhood of the support of T, then

$$\hat{T}(k) = (2\pi)^{-n/2} T(\psi e^{-ik\cdot x})$$

Proof By Theorem IX.4c and the Fourier inversion formula we have $\widehat{fT} = (2\pi)^{-n/2} \hat{f} * \hat{T}$. Thus $\widehat{fT} \in O_M^n$ and

$$\begin{aligned}\widehat{fT}(k) &= (2\pi)^{-n/2} \hat{T}(\tilde{\hat{f}}_k) \\ &= (2\pi)^{-n/2} T(e^{-ik\cdot x} f)\end{aligned}$$ ∎

We remark that one can also define the convolution of a distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ with an $f \in \mathscr{D}(\mathbb{R}^n)$ by $(T * f)(y) = T(\tilde{f}_y)$. A proof similar to the proof of Theorem IX.4 shows that $T * f$ is a (not necessarily polynomially bounded) C^∞ function and that (IX.3) holds.

We have already introduced the term "approximate identity" in Section VIII.1; we now define it formally.

Definition Let $j(x)$ be a positive C^∞ function whose support lies in the sphere of radius one about the origin in $\mathbb{R}^n$ and which satisfies $\int j(x)\, dx = 1$. The sequence of functions $j_\varepsilon(x) = \varepsilon^{-n} j(x/\varepsilon)$ is called an **approximate identity.**

Proposition Suppose $T \in \mathscr{S}'(\mathbb{R}^n)$ and let $j_\varepsilon(x)$ be an approximate identity. Then $T * j_\varepsilon \to T$ weakly as $\varepsilon \to 0$.

Proof If $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $(T * j_\varepsilon)(\varphi) = T(\tilde{j}_\varepsilon * \varphi)$, so it is sufficient to show that $\tilde{j}_\varepsilon * \varphi \xrightarrow{\mathscr{S}(\mathbb{R}^n)} \varphi$. To do this it is sufficient to show that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \to \hat{\varphi}$. Since $\hat{j}_\varepsilon(\lambda) = \hat{j}(\varepsilon\lambda)$ and $\hat{j}(0) = (2\pi)^{-n/2}$, it follows that $(2\pi)^{n/2} \hat{j}_\varepsilon(x)$ converges to 1 uniformly on compact sets and is uniformly bounded. Similarly, $D^\alpha \hat{j}_\varepsilon$ converges uniformly to zero. We conclude that $(2\pi)^{n/2} \hat{j}_\varepsilon \hat{\varphi} \to \hat{\varphi}$. ∎

IX.2 The range of the Fourier transform: Classical spaces

We have defined the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$. In this section, Section IX.3, and Section IX.9, we investigate the range of the Fourier transform when it is restricted to various subsets of $\mathscr{S}'(\mathbb{R}^n)$. These

questions are natural and have historical interest, but more important, characterizing the range of the Fourier transform is very useful. One is often able to obtain information about the Fourier transform of a function and one would like to know what this says about the function itself. We begin with two theorems which follow easily from the work that we have already done in Section IX.1.

Theorem IX.6 (the Plancherel theorem) The Fourier transform extends uniquely to a unitary map of $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^n)$. The inverse transform extends uniquely to its adjoint.

Proof The corollary to Theorem IX.1 states that if $f \in \mathscr{S}(\mathbb{R}^n)$, then $\|f\|_2 = \|\hat{f}\|_2$. Since $\mathscr{F}[\mathscr{S}] = \mathscr{S}$, $\mathscr{F}$ is a surjective isometry on $L^2(\mathbb{R}^n)$. ∎

Theorem IX.7 (the Riemann–Lebesgue lemma) The Fourier transform extends uniquely to a bounded map from $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$, the continuous functions vanishing at ∞.

Proof For $f \in \mathscr{S}(\mathbb{R}^n)$, we know that $\hat{f} \in \mathscr{S}(\mathbb{R}^n)$ and thus $\hat{f} \in C_\infty(\mathbb{R}^n)$. The estimate

$$\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$$

is trivial. The Fourier transform is thus a bounded linear map from a dense set of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. By the B.L.T. theorem, $\hat{}$ extends uniquely to a bounded linear transformation of $L^1(\mathbb{R}^n)$ into $C_\infty(\mathbb{R}^n)$. ∎

We remark that the Fourier transform takes $L^1(\mathbb{R}^n)$ into, but not onto $C_\infty(\mathbb{R}^n)$ (Problem 16).

A simple argument with test functions shows that the extended transform on $L^1(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$ is the restriction of the transform on $\mathscr{S}'(\mathbb{R}^n)$, but it is useful to have an explicit integral representation. For $f \in L^1(\mathbb{R}^n)$, this is easy since we can find $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\|f - f_m\|_1 \to 0$. Then, for each λ,

$$\begin{aligned}\hat{f}(\lambda) &= \lim_{m\to\infty}(\hat{f}_m(\lambda)) \\ &= \lim_{m\to\infty}\left\{\frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f_m(x)\,dx\right\} \\ &= \frac{1}{(2\pi)^{n/2}}\int_{\mathbb{R}^n} e^{-i\lambda\cdot x} f(x)\,dx\end{aligned}$$

So, the Fourier transform of a function in $L^1(\mathbb{R}^n)$ is given by the usual formula.

Next, suppose $f \in L^2(\mathbb{R}^n)$ and let

$$\chi_R(x) = \begin{cases} 1 & |x| \leq R \\ 0 & |x| > R \end{cases}$$

Then $\chi_R f \in L^1(\mathbb{R}^n)$ and $\chi_R f \xrightarrow[R\to\infty]{L^2} f$, so by the Plancherel theorem $\widehat{\chi_R f} \xrightarrow[R\to\infty]{L^2} \hat{f}$. For $\chi_R f$ we have the usual formula; thus

$$\hat{f}(\lambda) = \underset{R\to\infty}{\text{l.i.m.}}(2\pi)^{-n/2}\int_{|x|\leq R} e^{-i\lambda\cdot x} f(x)\,dx$$

where by "l.i.m." we mean the limit in the L^2-norm. Sometimes we will dispense with $|x| \leq R$ and just write

$$\hat{f}(\lambda) = \text{l.i.m.}(2\pi)^{-n/2}\int e^{-i\lambda\cdot x} f(x)\,dx$$

for functions $f \in L^2(\mathbb{R}^n)$.

We have proven above that $L^2(\mathbb{R}^n) \xrightarrow{\hat{}} L^2(\mathbb{R}^n)$ and $L^1(\mathbb{R}^n) \xrightarrow{\hat{}} L^\infty(\mathbb{R}^n)$ and in both cases $\hat{}$ is a bounded operator. It is exactly in situations like this that one can use the interpolation theorems which we will prove in the Appendix to Section 4.

Theorem IX.8 (Hausdorff–Young inequality) Suppose $1 \leq q \leq 2$, and $p^{-1} + q^{-1} = 1$. Then the Fourier transform is a bounded map of $L^q(\mathbb{R}^n)$ to $L^p(\mathbb{R}^n)$ and its norm is less than or equal to $(2\pi)^{n(1/2-1/q)}$.

Proof We use the Riesz–Thorin theorem (Theorem IX.17) with $q_0 = 2 = p_0$, $p_1 = \infty$, and $q_1 = 1$. Since $\|\hat{f}\|_2 = \|f\|_2$ and $\|\hat{f}\|_\infty \leq (2\pi)^{-n/2}\|f\|_1$, we conclude that $\|\hat{f}\|_{p_t} \leq C_t\|f\|_{q_t}$ where $p_t^{-1} = (1-t)/2$, $q_t^{-1} = (1-t)/2 + t = 1 - p_t^{-1}$, and $\log C_t = t\log(2\pi)^{-n/2}$. ∎

* * *

We now come to another natural question. What are the Fourier transforms of the finite positive measures on $\mathbb{R}^n$? Suppose that we define

$$\hat{\mu}(\lambda) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{-i\lambda\cdot x}\,d\mu(x)$$

Then, if $\varphi \in \mathscr{S}(\mathbb{R}^n)$,

$$\int_{\mathbb{R}^n} \hat{\mu}(\lambda)\varphi(\lambda)\, d\lambda = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x}\, d\mu(x) \right) \varphi(\lambda)\, d\lambda$$

$$= (2\pi)^{-n/2} \int_{\mathbb{R}^n} \left(\int_{\mathbb{R}^n} e^{-i\lambda \cdot x} \varphi(\lambda)\, d\lambda \right) d\mu(x)$$

$$= \int_{\mathbb{R}^n} \hat{\varphi}(x)\, d\mu(x)$$

so this definition coincides with the restriction of the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ to the positive measures. Suppose $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ and $\xi = \langle \xi_1, \xi_2, \ldots, \xi_N \rangle \in \mathbb{C}^N$. Then

$$\sum_{i,j=1}^{N} \hat{\mu}(\lambda_i - \lambda_j)\bar{\xi}_j \xi_i = \int \left| \sum_{i=1}^{N} \xi_i e^{-i\vec{\lambda}_i \cdot \mathbf{x}} \right|^2 d\mu(\mathbf{x}) \geq 0$$

This shows that the function $\hat{\mu}(\lambda)$ has the property that for any $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$, $\{\hat{\mu}(\lambda_i - \lambda_j)\}$ is the matrix of a positive operator on $\mathbb{C}^N$. Furthermore, by the dominated convergence theorem, $\hat{\mu}$ is continuous, and since

$$|\hat{\mu}(\lambda)| \leq (2\pi)^{-n/2} \int_{\mathbb{R}^n} |e^{-i\lambda \cdot \mathbf{x}}|\, d\mu(\mathbf{x})$$

$$= (2\pi)^{-n/2} \mu(\mathbb{R}^n)$$

$\hat{\mu}(\cdot)$ is also bounded.

Definition A complex-valued, bounded, continuous function f on $\mathbb{R}^n$ that has the property that $\{f(\lambda_i - \lambda_j)\}_{i,j}$ is a positive matrix on $\mathbb{C}^N$ for each N and all $\lambda_1, \ldots, \lambda_N \in \mathbb{R}^n$ is called a **function of positive type**.

There are three properties of functions of positive type which follow easily from the definition. Letting $N = 1$, $x \in \mathbb{R}^N$,

$$(1) \quad f(0) \geq 0$$

since $f(0)$ is a positive operator on $\mathbb{C}^1$. Letting $N = 2$, and choosing $\lambda_1 = x$, $\lambda_2 = 0$, we see that the matrix

$$\begin{pmatrix} f(0) & f(x) \\ f(-x) & f(0) \end{pmatrix}$$

must be positive and therefore self-adjoint with positive determinant. This implies that

$$(2) \quad f(x) = \overline{f(-x)}$$
$$(3) \quad |f(x)| \leq f(0)$$

Notice that in proving these three properties we did not use the fact that $f(x)$ is bounded, so we could have left out the word *bounded* in the definition and recovered boundedness from (3) above. It is clear that any convex combinations or scalar multiples of functions of positive type again give functions of positive type, so these functions form a cone.

Theorem IX.9 (Bochner's theorem) The set of Fourier transforms of the finite, positive measures on $\mathbb{R}^n$ is exactly the cone of functions of positive type.

Proof We do not give Bochner's original proof but rather an easy, interesting argument based on Stone's theorem. We have already shown that the Fourier transforms of finite positive measures are functions of positive type. We need to prove the converse. Suppose f is of positive type. Let $\mathscr{K}$ denote the set of complex-valued functions on $\mathbb{R}^n$ which vanish except at a finite number of points. Then

$$(\psi, \varphi)_f = \sum_{\mathbf{x}, \mathbf{y} \in \mathbb{R}^n} f(\mathbf{x} - \mathbf{y})\overline{\psi(\mathbf{x})}\varphi(\mathbf{y})$$

has all the properties of a well-defined inner product except that we may have $(\varphi, \varphi)_f = 0$ for some $\varphi \neq 0$. If we let $\mathscr{N}$ be the set of such φ, then $\mathscr{K}/\mathscr{N}$ is a well-defined pre-Hilbert space under $(\cdot, \cdot)_f$. Suppose that $\mathbf{t} \in \mathbb{R}^n$ and define $U_\mathbf{t}$ on $\mathscr{K}$ by $(U_\mathbf{t}\varphi)(\mathbf{x}) = \varphi(\mathbf{x} - \mathbf{t})$. Since $U_\mathbf{t}$ preserves the form $(\cdot, \cdot)_f$, it takes equivalence classes into equivalence classes and thus restricts to an isometry on $\mathscr{K}/\mathscr{N}$. Since the same is true of $U_{-\mathbf{t}}$, this isometry has dense range and thus extends to a unitary operator $\tilde{U}_\mathbf{t}$ on $\mathscr{H} = \overline{\mathscr{K}/\mathscr{N}}$. Furthermore, $\tilde{U}_{\mathbf{t}+\mathbf{s}} = \tilde{U}_\mathbf{t}\tilde{U}_\mathbf{s}$, $\tilde{U}_0 = I$, and because of the continuity of f, $\tilde{U}_\mathbf{t}$ is strongly continuous. Thus the map $\mathbf{t} \to \tilde{U}_\mathbf{t}$ satisfies the hypotheses of Theorem VIII.12 (the generalization of Stone's theorem). Therefore, there is a projection-valued measure P_λ, on $\mathbb{R}^n$ so that

$$(\varphi, \tilde{U}_\mathbf{t}\psi)_f = \int_{\mathbb{R}^n} e^{i\mathbf{t} \cdot \lambda}\, d(\varphi, P_\lambda \psi)_f$$

Let $\tilde{\varphi}_0$ denote the equivalence class containing the function

$$\varphi_0(\mathbf{x}) = \begin{cases} 1, & x = 0 \\ 0, & x \neq 0 \end{cases}$$

Then

$$f(\mathbf{t}) = \tilde{U}_\mathbf{t}\tilde{\varphi}_0, \tilde{\varphi}_0)_f = (\tilde{\varphi}_0, \tilde{U}_{-\mathbf{t}}\tilde{\varphi}_0)_f = \int e^{-i\mathbf{t} \cdot \lambda}\, d(\tilde{\varphi}_0, P_\lambda \tilde{\varphi}_0)_f$$

so we have displayed f as the Fourier transform of a finite positive measure. ∎

The notion of positive type may be generalized to distributions. If $f(x)$ is a bounded continuous function, then $f(x)$ will be of positive type if and only if

$$\int\int f(x-y)\overline{\varphi(y)}\varphi(x)\,dx\,dy \geq 0 \tag{IX.4}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. To see this one need only approximate the integral in (IX.4) by a Riemann sum. This condition can be rewritten as

$$\iint f(\tau)\overline{\varphi(x-\tau)}\varphi(x)\,d\tau\,dx = \int f(\tau)(\bar{\tilde{\varphi}} * \varphi)(\tau)\,d\tau \geq 0 \tag{IX.5}$$

where $\tilde{\varphi}$ is the function $\tilde{\varphi}(x) = \varphi(-x)$. This suggests the following definition.

Definition A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is said to be of **positive type** if $T(\bar{\tilde{\varphi}} * \varphi) \geq 0$ for all $\varphi \in \mathscr{D}(\mathbb{R}^n)$.

The following generalization of Bochner's theorem is due to Schwartz. This theorem is particularly interesting since it implies that certain ordinary distributions must be tempered. The proof is sketched in Problem 20 (or see the Notes for a reference).

Theorem IX.10 (the Bochner–Schwartz theorem) A distribution $T \in \mathscr{D}'(\mathbb{R}^n)$ is a distribution of positive type if and only if $T \in \mathscr{S}'(\mathbb{R}^n)$ and T is the Fourier transform of a positive measure of at most polynomial growth.

If $f(x)$ is a function of positive type, then this theorem implies that the weak derivatives $(-\Delta)^m f$ are all distributions of positive type. For $\hat{f} = \mu$, a finite measure by Theorem IX.9, and $\widehat{(-\Delta)^m f} = |x|^{2m}\mu$, a positive measure of polynomial growth.

Finally, we determine which bounded measurable functions are distributions of positive type. A bounded measurable function f on $\mathbb{R}^n$ is said to be of **weak positive type** if (IX.4) holds. Since (IX.5) follows from (IX.4), the distribution

$$T_f(\varphi) = \int f(x)\varphi(x)\,dx$$

is of positive type and therefore $\hat{T}_f = \mu$, a polynomially bounded positive measure. If $j_\varepsilon(x)$ is an approximate identity that is symmetric about the origin, then

$$\begin{aligned}\|f\|_\infty \geq T_f(j_\varepsilon * j_\varepsilon) &= \hat{T}_f(\widetilde{(j_\varepsilon * j_\varepsilon)}) \\ &= (2\pi)^{n/2}\mu(|\check{j}_\varepsilon(x)|^2) \\ &= (2\pi)^{n/2}\int |\check{j}_\varepsilon(x)|^2\,d\mu(x)\end{aligned}$$

On each compact subset of $\mathbb{R}^n$, $\check{j}_\varepsilon(x)$ converges uniformly to $(2\pi)^{-n/2}$ as $\varepsilon \to 0$, so the μ-measure of any compact set is less than $(2\pi)^{n/2}\|f\|_\infty$, so μ is finite.

We now come to the interesting point. Since μ is finite, its Fourier transform is a continuous function of positive type. Since μ and f must coincide a.e., we have proven:

Proposition A bounded function of weak positive type is equal almost everywhere to a continuous function of positive type.

IX.3 The range of the Fourier transform: Analyticity

In this section we investigate the connection between the decay properties of a function or distribution at infinity and the analyticity properties of its Fourier transform. The most extreme form of decay at infinity is to have compact support. We will prove the Paley–Wiener and Schwartz theorems which characterize explicitly the Fourier transforms of C^∞ functions and distributions with compact support. We then state two theorems relating exponential decay to analyticity properties of the Fourier transform. We close the section by characterizing the Fourier transforms of tempered distributions whose supports lie in symmetric cones. There are many other theorems of this genre; some of them are discussed in the Notes.

Suppose that $f \in C_0^\infty(\mathbb{R}^n)$. Then for all $\zeta = \langle \zeta_1, \ldots, \zeta_n \rangle \in \mathbb{C}^n$, the integral

$$\hat{f}(\zeta) = (2\pi)^{-n/2}\int e^{-i\zeta\cdot x} f(x)\,dx$$

is well defined. Furthermore, $\hat{f}(\zeta)$ is an entire analytic function of the n complex variables $\zeta_1, \zeta_2, \ldots, \zeta_n$ since we can differentiate under the

integral sign. In addition, if the support of f is contained in the sphere of radius R, then an integration by parts yields

$$\prod_{i=1}^{n}(i\zeta_i)^{\alpha}\hat{f}(\zeta) = (2\pi)^{-n/2}\int_{|x|\le R} e^{-i\zeta\cdot x}D^{\alpha}f(x)\,dx$$

Taking the absolute value of both sides and using the fact that $\hat{f}(\zeta)$ is bounded on the set $\{\zeta \mid |\operatorname{Im}\zeta| < \varepsilon\}$, we easily conclude that for each N,

$$|\hat{f}(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \qquad \text{for all } \zeta \in \mathbb{C}^n$$

where C_N is a constant that depends on N and f. The interesting fact is that these estimates are not only necessary but also sufficient for f to be in $C_0^{\infty}(\mathbb{R}^n)$.

Theorem IX.11 (the Paley–Wiener theorem) An entire analytic function of n complex variables $g(\zeta)$ is the Fourier transform of a $C_0^{\infty}(\mathbb{R}^n)$ function with support in the ball $\{x \mid |x| \le R\}$ if and only if for each N there is a C_N so that

$$|g(\zeta)| \le \frac{C_N e^{R|\operatorname{Im}\zeta|}}{(1+|\zeta|)^N} \tag{IX.6}$$

for all $\zeta \in \mathbb{C}^n$.

Proof We have already proven the "only if" part. Suppose that g is entire and satisfies estimates of the form (IX.6). Let $\zeta = \lambda + i\eta$, where $\lambda, \eta \in \mathbb{R}^n$. Then for each η, $g(\lambda + i\eta)$ is in $\mathscr{S}(\mathbb{R}^n)$ as a function of λ, since the derivatives fall off polynomially by (IX.6) and the Cauchy formula. Let

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{ix\cdot\lambda}g(\lambda)\,d\lambda \tag{IX.7}$$

Then by Theorem IX.1, $f \in \mathscr{S}(\mathbb{R}^n)$ and $g(\lambda) = \hat{f}(\lambda)$. We want to show that $f(x)$ has support in the ball of radius R. Because of the estimates (IX.6) and Cauchy's theorem, we can shift the region of integration in (IX.7) so that

$$f(x) = (2\pi)^{-n/2}\int_{\mathbb{R}^n} e^{i(\lambda+i\eta)\cdot x}g(\lambda+i\eta)\,d\lambda \tag{IX.8}$$

Thus, by (IX.6)

$$|f(x)| \le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda+i\eta|)^N}\,d\lambda$$

$$\le e^{R|\eta|-x\cdot\eta}(2\pi)^{-n/2}\int \frac{C_N}{(1+|\lambda|)^N}\,d\lambda$$

where we have chosen N large enough so that the integral on the right is finite. Now, $f(x)$ does not depend on η, so if we let $\eta \to \infty$ in an appropriate direction, we conclude that $|f(x)| = 0$ if $|x| > R$. ∎

This theorem has a natural generalization to the distributions with compact support. Recall that a distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has support in a closed set K if and only if $T(\varphi) = 0$ for every test function φ with support in $\mathbb{R}^n \backslash K$. If K is compact, then T is said to have **compact support**. The set of distributions with compact support is the dual space of $\mathscr{E}(\mathbb{R}^n)$ (see Problems 39 and 40 of Chapter V).

Theorem IX.12 A distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support if and only if $\hat{T}$ has an analytic continuation to an entire analytic function of n variables $\hat{T}(\zeta)$ that satisfies

$$|\hat{T}(\zeta)| \le C(1+|\zeta|)^N e^{R|\operatorname{Im}\zeta|} \tag{IX.9}$$

for all $\zeta \in \mathbb{C}^n$ and some constants C, N, R. Moreover, if (IX.9) holds, the support of T is contained in the ball of radius R.

Proof Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ has compact support and let φ be a $C_0^{\infty}(\mathbb{R}^n)$ function which is equal to one on the support of T. Define $F(\zeta) = T[(2\pi)^{-n/2}e^{-i\zeta\cdot x}\varphi(x)]$. By Theorem IX.5, $F(\lambda + i0)$ is the Fourier transform of T. Furthermore, since

$$\left(\frac{\exp(-i(x_j(\zeta_j+h_j)+\sum_{k\ne j}\zeta_k x_k))\varphi(x) - e^{-i\zeta\cdot x}\varphi(x)}{h_j}\right)$$

$$\xrightarrow{\mathscr{S}(\mathbb{R}^n)} -ix_j e^{-i\zeta\cdot x}\varphi(x)$$

and $T \in \mathscr{S}'(\mathbb{R}^n)$, $F(\zeta)$ is differentiable in the complex sense in each variable and is thus entire.

Since $T \in \mathscr{S}'(\mathbb{R}^n)$,

$$|T(f)| \le C_1 \sum_{\substack{|\alpha|\le N\\ |\beta|\le N}} \|x^{\alpha}D^{\beta}f\|_{\infty}$$

for some N and C_1 and all $f \in \mathscr{S}(\mathbb{R}^n)$. Thus, if φ has support in the sphere of radius R, then

$$|F(\zeta)| \le C_2(1+R^n)(1+|\zeta|^N)e^{|\operatorname{Im}\zeta|R}$$

Conversely, suppose that $F(\zeta)$ is an entire function satisfying the estimate (IX.9). Then $F(\lambda + i0) \in \mathscr{S}'(\mathbb{R}^n)$, so it is the Fourier transform of some $T \in \mathscr{S}'(\mathbb{R}^n)$. Let $j_{\varepsilon}(x)$ be an approximate identity. Then by Theorem IX.4,

$\widehat{T * j_\varepsilon} = (2\pi)^{-n/2}\hat{j}_\varepsilon(\lambda)F(\lambda)$. Since j_ε has compact support in $\{x \mid |x| \leq \varepsilon\}$, we know by the Paley–Wiener theorem, that for each M we can find a constant C_M so that

$$|\hat{j}_\varepsilon(\zeta)| \leq \frac{C_M}{(1 + |\zeta|)^{N+M}} e^{\varepsilon|\operatorname{Im}\zeta|}$$

Therefore

$$|(2\pi)^{-n/2}\hat{j}_\varepsilon(\zeta)F(\zeta)| \leq \frac{C_M C e^{(R+\varepsilon)|\operatorname{Im}\zeta|}}{(1 + |\zeta|)^N}$$

which implies (again by the Paley–Wiener theorem) that the support of $T * j_\varepsilon$ is contained in the sphere of radius $R + \varepsilon$. Since ε is arbitrary and $(T * j_\varepsilon) \to T$ weakly, we conclude that the support of T is contained in the sphere of radius R about the origin. ∎

One natural way to extend the above theorems is to replace "compact support" with some weaker notion of decay at infinity. The following pair of theorems (whose proofs are outlined in Problem 76) will be used in Chapter XIII to prove the exponential decay of bound states of atomic Hamiltonians.

Theorem IX.13 Let f be in $L^2(\mathbb{R}^n)$. Then $e^{b|x|}f \in L^2(\mathbb{R}^n)$ for all $b < a$ if and only if $\hat{f}$ has an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ with the property that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{f}(\cdot + i\eta) \in L^2(\mathbb{R}^n)$ and for any $b < a$

$$\sup_{|\eta| \leq b} \|\hat{f}(\cdot + i\eta)\|_2 < \infty$$

Theorem IX.14 Let T be in $\mathscr{S}'(\mathbb{R}^n)$. Suppose that $\hat{T}$ is a function with an analytic continuation to the set $\{\zeta \mid |\operatorname{Im}\zeta| < a\}$ for some $a > 0$. Suppose further that for each $\eta \in \mathbb{R}^n$ with $|\eta| < a$, $\hat{T}(\cdot + i\eta) \in L^1(\mathbb{R}^n)$ and for any $b < a$, $\sup_{|\eta| < b} \|\hat{T}(\cdot + i\eta)\|_1 < \infty$. Then T is a bounded continuous function and for any $b < a$, there is a constant C_b so that

$$|T(x)| \leq C_b e^{-b|x|}$$

The next natural question to ask is what are the analyticity properties of a function or distribution with support on a half-line, half-space, or in general in a cone? As a simple example, consider the Fourier transform $\hat{f}$ of

a function $f \in \mathscr{S}(\mathbb{R})$ which has support contained in $[0, \infty)$. The reader can easily verify that

$$\hat{f}(\lambda - i\eta) = (2\pi)^{-1/2} \int e^{-i(\lambda - i\eta)\cdot x} f(x)\, dx \tag{IX.10}$$

is a well-defined analytic function in the open lower half-plane (i.e. for $\eta > 0$) and that $\hat{f}(\cdot - i\eta) \xrightarrow{\mathscr{S}(\mathbb{R})} \hat{f}$ as $\eta \downarrow 0$. That is, $\hat{f}$, which need not be real analytic, is the "boundary value" of an analytic function in the lower half-plane. The study of the Fourier transforms of functions and distributions with supports in half-spaces dates back to the classical investigations of the Laplace transform and has played an important role in modern analysis. The main ideas and techniques are similar to those used above in Theorem IX.11 and Theorem IX.12. However, an additional difficulty arises since one must specify in what sense the Fourier transform is the "boundary value" of the analytic function. There is a wide range of such theorems; we will discuss one which we will use in Section IX.8 in our study of quantum field theory. Some of the others are briefly discussed in the Notes.

Definition Let $a \in \mathbb{R}^n$, $|a| = 1$, and $\theta \in (0, \pi/2)$. Then

$$\Gamma_{a,\theta} = \{\xi \in \mathbb{R}^n \mid \xi \cdot a > |\xi| \cos\theta\}$$

is called the **cone about a of opening angle θ**. The cone $\Gamma^*_{a,\theta} \equiv \Gamma_{a,\pi/2-\theta}$ is called the **dual cone**. When no confusion arises, we will drop the subscripts and just refer to Γ and Γ^*.

The dual cone Γ^* will either contain Γ (as in Figure IX.1) or be contained in Γ. Notice that Γ^* is the interior of the intersection of the half-spaces $\{\eta \mid \eta \cdot \xi > 0\}$ for $\xi \in \Gamma$. If Γ is the open forward light cone in $\mathbb{R}^4$ (with the velocity of light equal to one), then Γ^* is also the open forward light cone. Given an open cone $C \subset \mathbb{R}^n$, we will denote by $\mathbb{R}^n - iC$ the open region of those $\zeta = \langle \lambda_1 - i\eta_1, \lambda_2 - i\eta_2, \ldots, \lambda_n - i\eta_n \rangle \in \mathbb{C}^n$ so that $\lambda = \langle \lambda_1, \ldots, \lambda_n \rangle \in \mathbb{R}^n$ and $\eta = \langle \eta_1, \ldots, \eta_n \rangle \in C$. $\mathbb{R}^n - iC$ is called the **tube with base C**.

We can now say what we mean by "boundary value."

Definition Let $S \in \mathscr{S}'(\mathbb{R}^n)$ and suppose $F(\zeta)$ is a function analytic in $\mathbb{R}^n - iC$ for some cone C. Suppose that for each fixed $\eta_0 \in C$, $F(\lambda - i\eta_0)$ is a tempered distribution (i.e. has at most polynominal growth in λ) and that as $t \downarrow 0$ in $\mathbb{R}$

$$\int_{\mathbb{R}^n} F(\lambda - it\eta_0)\varphi(\lambda)\, d\lambda \to S(\varphi)$$

for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. Then S is said to be the (distributional) **boundary value of F in the sense of $\mathscr{S}'(\mathbb{R}^n)$**.

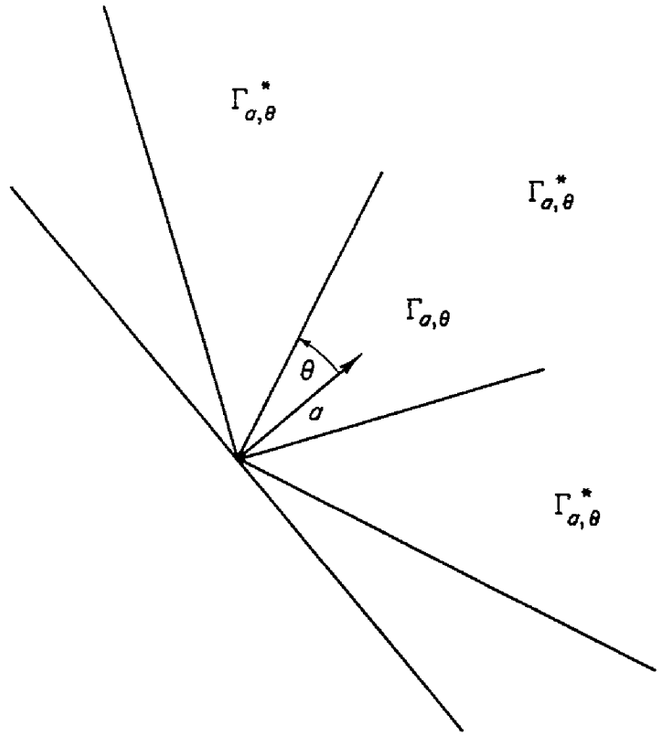


FIGURE IX.1 The cones $\Gamma_{a,\theta}$ and $\Gamma^*_{a,\theta}$.

Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ and that the support of T is contained in $\Gamma_{a,\theta}$ for some $a \in \mathbb{R}^n$ and $\theta \in (0, \pi/2)$. If T is given by a function $T(x)$, then we can directly extend $\hat{T}$ to the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ by

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} \int_{\Gamma_{a,\theta}} e^{-i(\lambda - i\eta)\cdot x} T(x)\, dx$$

For $\eta \in \Gamma^*_{a,\theta}$, the integral makes sense since

$$|e^{-i(\lambda - i\eta)\cdot x}| = e^{-|\eta||x|\cos(\eta, x)} \leq e^{-|x|\, d(\eta)}$$

where $d(\eta) \equiv |\eta| \min_{x \in \partial\Gamma_{a,\theta}} \cos(\eta, x) = \operatorname{dist}(\eta, \partial\Gamma^*_{a,\theta})$; see Figure IX.1. Since $T(x)$ is polynomially bounded, the presence of the factor $e^{-|x|\, d(\eta)}$ means that we may differentiate under the integral sign. We conclude that $\hat{T}(\lambda - i\eta)$ is analytic in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ since it is infinitely differentiable in the complex sense. Furthermore, if $\varphi \in \mathscr{S}(\mathbb{R}^n)$, and $\eta_0 \in \Gamma^*_{a,\theta}$, then

$$\int_{\mathbb{R}^n} \hat{T}(\lambda - it\eta_0)\varphi(\lambda)\, d\lambda = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \int_{\Gamma_{a,\theta}} e^{-i(\lambda - it\eta_0)\cdot x} \varphi(\lambda) T(x)\, dx\, d\lambda$$

$$= \int_{\Gamma_{a,\theta}} e^{-t\eta_0 \cdot x} \hat{\varphi}(x) T(x)\, dx$$

$$\xrightarrow[t \downarrow 0]{} \int_{\Gamma_{a,\theta}} \hat{\varphi}(x) T(x)\, dx = \hat{T}(\varphi)$$

by the dominated convergence theorem. Thus, $\hat{T}$ is the boundary value of $\hat{T}(\lambda - i\eta)$ in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$.

If T is not a function but is of the form $P(D)G$ where G is a polynomially bounded continuous function with support in $\bar{\Gamma}_{a,\theta}$, then we can define

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} P(i(\lambda - i\eta)) \int_{\Gamma_{a,\theta}} e^{-i(\lambda - i\eta)\cdot x} G(x)\, dx$$

In the same way as above, one can then show that $\hat{T}(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and that $\hat{T}$ is the boundary value of $\hat{T}(\lambda - i\eta)$. Thus, we wish to prove that *every* tempered distribution T with support in a cone can be written $T = P(D)G$ for some partial differential operator $P(D)$ and some polynomially bounded continuous function G *with support in the cone.* To see that this is a strong statement the reader should recall that the analogous statement for compact sets (rather than cones) is false. For example, the delta function cannot be written as $P(D)G$ where G has support at the origin.

Theorem IX.15 (Bros–Epstein–Glaser lemma) Let Γ be a proper open convex cone in $\mathbb{R}^n$ and let $T \in \mathscr{S}'(\mathbb{R}^n)$ have support in $\bar{\Gamma}$. Then there exists a polynomially bounded continuous function G *with support in* $\bar{\Gamma}$ and a partial differential operator $P(D)$ so that $T = P(D)G$.

Proof Let $\{\mathbf{e}_i\}_{i=1}^n$ be a basis for $\mathbb{R}^n$ consisting of vectors in Γ. Every vector $x \in \mathbb{R}^n$ may be uniquely written $x = \sum_{i=1}^n y_i \mathbf{e}_i$ so that we may use $\{y_i\}_{i=1}^n$ as coordinates for $\mathbb{R}^n$. Define

$$F_m(y_1, \ldots, y_n) = (m!)^{-n} y_1^m y_2^m \cdots y_n^m \theta(y_1) \cdots \theta(y_n)$$

where θ is the characteristic function of $\{x \mid x \in \mathbb{R},\ x \geq 0\}$. Then $F_m \in C^{m-1}(\mathbb{R}^n)$ and F_m has support in $\bar{\Gamma}$. Furthermore, if $Q(D) = \partial^n/\partial y_1 \cdots \partial y_n$, then $Q(D)^{m+1} F_m = \delta$ as the reader can easily check. We will show that for m sufficiently large, the convolution $T * F_m$ is a well-defined continuous function with support in $\bar{\Gamma}$ and that $Q(D)^{m+1}(T * F_m) = T * Q(D)^{m+1} F_m = T * \delta = T$.

If $b \in \Gamma$, then $\bar{\Gamma}$ is contained in the interior of $\bar{\Gamma} - b$ so we may find a C^∞ function ψ that equals one on $\bar{\Gamma}$ and has support in $\bar{\Gamma} - b$ (see Figure IX.2). Since $T \in \mathscr{S}'(\mathbb{R}^n)$, there is an N so that

$$|T(\varphi)| = |T(\psi\varphi)| \leq C_1 \sum_{\substack{|\alpha| \leq N \\ |\beta| \leq N}} \|x^\alpha D^\beta(\psi\varphi)\|_\infty$$

$$\leq C_2 \sum_{\substack{|\alpha| \leq N \\ |\alpha| \leq N}} \left(\sup_{x \in \bar{\Gamma} - b} |x^\alpha D^\beta \varphi(x)| \right) \equiv |||\varphi|||_b$$

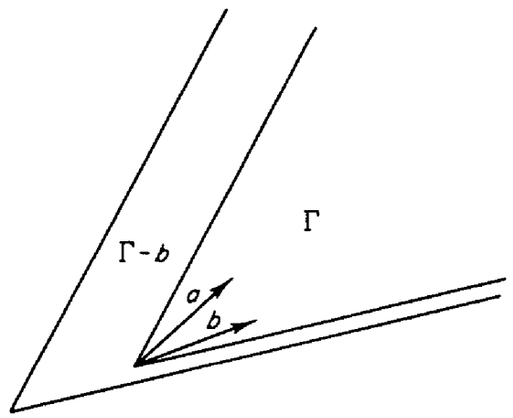


FIGURE IX.2 The cone $\Gamma - b$.

Thus, T has a unique extension, continuous in $|||\cdot|||_b$, to those C^N functions f for which (supp f) $\cap$ $(\bar{\Gamma} - b)$ is compact.

Choose $m = N + 1$ and for $y \in \mathbb{R}^n$ define $\tilde{F}_{N+1;\,y}(x) = F_{N+1}(y - x)$. Then $\tilde{F}_{N+1;\,y}$ is a C^N function and (supp $\tilde{F}_{N+1;\,y}$) $\cap$ $\bar{\Gamma} - b$ is compact (see Figure IX.3). Further, the map $y \to \tilde{F}_{N+1;\,y}$ is $|||\cdot|||_b$-continuous and polynomially bounded in y (see Figure IX.2). Thus, $G(y) = T * F_{N+1}(y) \equiv T(\tilde{F}_{N+1;\,y})$ is a polynomially bounded continuous function and supp $G \subset \bar{\Gamma}$ since

$$(\text{supp } \tilde{F}_{N+1;\,y}) \cap \Gamma = \varnothing \qquad \text{if } y \notin \bar{\Gamma}$$

Furthermore, if $f \in C_0^\infty(\mathbb{R}^n)$, then

$$(f * G)(y) = T((f * F_{N+1})^{\sim}_y) \tag{IX.11}$$

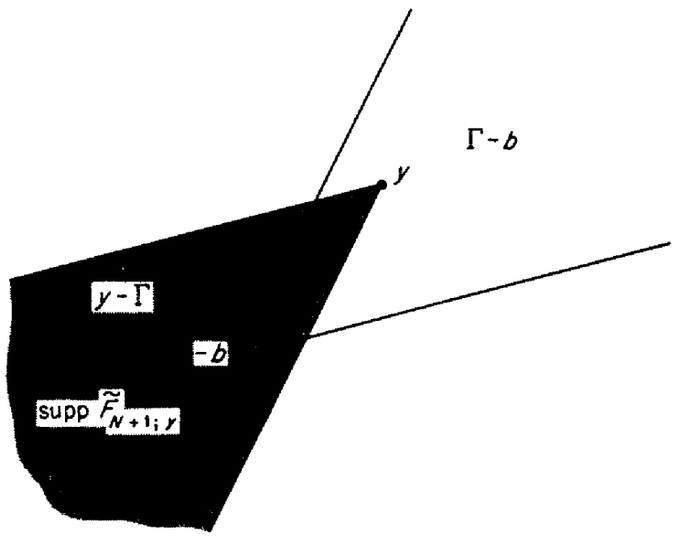


FIGURE IX.3 The support of $F_{N+1;\,y}$.

and

$$D^\alpha(f * G)(y) = T((D^\alpha f * F_{N+1})^{\sim}_y) \tag{IX.12}$$

These formulas are analogous to those in Theorem IX.4. Both may be proven by writing approximate Riemann sums for the integrals on the right and then observing that the approximate Riemann sums converge in $|||\cdot|||_b$. If we now let $j_\varepsilon(x)$ be an approximate identity, then by the proposition at the end of Section IX.1,

$$Q(D)^{N+2}G = \lim_{\varepsilon \downarrow 0} Q(D)^{N+2}(j_\varepsilon * G)$$

[by (IX.12)]

$$= \lim_{\varepsilon \downarrow 0} T((Q(D)^{N+2} j_\varepsilon * F_{N+1})^{\sim}_y)$$

(by Theorem IX.4)

$$= \lim_{\varepsilon \downarrow 0} T((j_\varepsilon * Q(D)^{N+2} F_{N+1})^{\sim}_y)$$

$$= \lim_{\varepsilon \downarrow 0} T((\check{j}_\varepsilon)_y)$$

$$= \lim_{\varepsilon \downarrow 0} j_\varepsilon * T = T \quad \blacksquare$$

Theorem IX.16 Let T be a tempered distribution with support in the cone $\bar{\Gamma}_{a,\theta}$, $a \in \mathbb{R}^n$, $0 < \theta < \pi/2$. Then $\hat{T}$ is the boundary value in the sense of $\mathcal{S}'(\mathbb{R}^n)$ of a function $\hat{T}(\lambda - i\eta)$ analytic in the tube $\mathbb{R}^n - i\Gamma^*_{a,\theta}$. Moreover, $\hat{T}(\lambda - i\eta)$ satisfies the estimate

$$|\hat{T}(\lambda - i\eta)| \leq |P(\lambda - i\eta)|(1 + [\text{dist}(\eta, \partial\Gamma^*_{a,\theta})]^{-N}) \tag{IX.13}$$

for a suitable polynomial P and positive integer N.

Conversely, suppose $F(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and satisfies the weaker estimates:

(i) For each $\eta_0 \in \Gamma^*_{a,\theta}$, there is a polynomial P_{η_0} in $2n$ variables so that

$$|F(\lambda - i(\eta_0 + \eta))| \leq |P_{\eta_0}(\lambda, \eta)|$$

for all $\lambda \in \mathbb{R}^n$ and $\eta \in \Gamma^*_{a,\theta}$.

(ii) There is an integer $r \geq 0$ so that for each $\eta_0 \in \Gamma^*_{a,\theta}$, there is a polynomial Q_{η_0} so that

$$|F(\lambda - it\eta_0)| \leq \frac{|Q_{\eta_0}(\lambda)|}{t^r}$$

for all $\lambda \in \mathbb{R}^n$ and $t \in (0, 1]$.

Then there is a tempered distribution T with support in the cone $\overline{\Gamma}_{a,\theta}$ so that $\hat{T}$ is the boundary value of $F(\lambda - i\eta)$ in the sense of $\mathscr{S}'(\mathbb{R}^n)$. Moreover, F can be recovered from T by the formula

$$F(\cdot - i\eta) = \widehat{e^{-\eta \cdot x} T} \tag{IX.14}$$

Proof Suppose that $T \in \mathscr{S}'(\mathbb{R}^n)$ and supp $T \subset \overline{\Gamma}_{a,\theta}$. By the Bros–Epstein–Glaser lemma, there is a polynomially bounded continuous function G with support in $\overline{\Gamma}_{a,\theta}$ so that $T = P(D)G$ for some partial differential operator $P(D)$. From the discussion before the lemma, we already know that $\hat{T}$ is the boundary value of the function

$$\hat{T}(\lambda - i\eta) = (2\pi)^{-n/2} P(i(\lambda - i\eta)) \int_{\mathbb{R}^n} e^{-i(\lambda - i\eta)\cdot x} G(x)\, dx$$

Thus,

$$|\hat{T}(\lambda - i\eta)| \leq (2\pi)^{-n/2} |P(i(\lambda - i\eta))| \int_{\mathbb{R}^n} e^{-|x|\, d(\eta)} |G(x)|\, dx$$

$$\leq C |P(i(\lambda - i\eta))| (1 + (d(\eta))^{-N})$$

since $G(x)$ has support in $\overline{\Gamma}_{a,\theta}$ and grows no worse at ∞ than $|x|^{N-n}$ for some N. This completes the proof in the first direction.

Conversely, we suppose that $F(\lambda - i\eta)$ is analytic in $\mathbb{R}^n - i\Gamma^*_{a,\theta}$ and that the estimates (i) and (ii) hold. The proof is in several steps. First we show that $F(\lambda - it\eta)$ has a tempered distribution $\hat{T}_\eta$ as boundary value as $t \downarrow 0$. Then we show that the limit is independent of η. Finally we show that T has support in $\overline{\Gamma}_{a,\theta}$.

For each fixed $\eta_0 \in \Gamma^*_{a,\theta}$, $0 < t \leq 1$, $F(\lambda - it\eta_0)$ is a well-defined distribution in $\mathscr{S}'(\mathbb{R}^n)$ which we denote by $\hat{T}_{t,\eta_0}$. Let $\psi \in \mathscr{S}(\mathbb{R}^n)$ and set

$$h(t) = \int_{\mathbb{R}^n} F(\lambda - it\eta_0)\psi(\lambda)\, d\lambda = \hat{T}_{t,\eta_0}(\psi)$$

Then,

$$\frac{d^j}{dt^j} h(t) = \int_{\mathbb{R}^n} F(\lambda - it\eta_0)\left(i\eta_0 \cdot \frac{\partial}{\partial\lambda}\right)^j \psi(\lambda)\, d\lambda$$

so,

$$\left|\frac{d^j}{dt^j} h(t)\right| \leq C \sup_\lambda \frac{|Q_{\eta_0}(\lambda)(1 + |\lambda|)^k|\,|(i\eta_0 \cdot \partial/\partial\lambda)^j \psi(\lambda)|}{t^r} \tag{IX.15}$$

where k has been chosen large enough so that $\int_{\mathbb{R}^n} (1 + |\lambda|)^{-k}\, d\lambda$ converges.

Let $p = r + 2$. Then, by the fundamental theorem of calculus,

$$h(t_1) = -\int_{t_1}^1 \int_{t_2}^1 \cdots \int_{t_{p-1}}^1 \left(\frac{d^p}{dt^p} h(t_p)\right) dt_p \cdots dt_2 + h(1) + \sum_{j=1}^{p-1} Q_j(t_1)\left(\frac{d^j}{dt_1^j} h\right)(1)$$

where the Q_j are suitable polynomials. The estimates (IX.15) show that the limit of $h(t_1)$ exists as $t_1 \downarrow 0$ and that each term in the limit is less than or equal to a constant times an $\mathscr{S}(\mathbb{R}^n)$-seminorm of ψ. Thus $F(\lambda - it\eta_0)$ converges in $\mathscr{S}'(\mathbb{R}^n)$ as $t \downarrow 0$ to a tempered distribution which we will denote by $\hat{T}_{0,\eta_0}$. Now suppose that $\eta_1, \eta_2 \in \Gamma^*_{a,\theta}$ and that $\check{\psi}(x)$ is in $C_0^\infty(\mathbb{R}^n)$. Then

$$\hat{T}_{t,\eta_1}(\psi) = \int_{\mathbb{R}^n} F(\lambda - it\eta_2 + it(\eta_2 - \eta_1))\psi(\lambda)\, d\lambda$$

$$= \int_{\mathbb{R}^n} F(\lambda - it\eta_2)\psi(\lambda - it(\eta_2 - \eta_1))\, d\lambda$$

$$= T_{t,\eta_2}(\widehat{e^{-t(\eta_2 - \eta_1)\cdot x}\check{\psi}(x)})$$

where we have used the fact that $\psi(\lambda)$ is entire and the estimates on $\psi(\lambda)$ in the Paley–Wiener theorem to shift the hyperplane of integration in the second step. Since $\check{\psi} \in C_0^\infty(\mathbb{R}^n)$, $\widehat{e^{-t(\eta_2 - \eta_1)\cdot x}\check{\psi}(x)} \xrightarrow{\mathscr{S}(\mathbb{R}^n)} \psi$ as $t \downarrow 0$. Thus by Theorem V.8,

$$\hat{T}_{t,\eta_2}(e^{-t(\eta_2 - \eta_1)\cdot x}\check{\psi}(x)) \to \hat{T}_{0,\eta_2}(\psi)$$

and therefore $\hat{T}_{0,\eta_1}(\psi) = \hat{T}_{0,\eta_2}(\psi)$. Since such ψ are dense in $\mathscr{S}(\mathbb{R}^n)$, $\hat{T}_{0,\eta_1} = \hat{T}_{0,\eta_2}$. Thus, the limit of $\hat{T}_{t,\eta_0}$ as $t \downarrow 0$ is independent of η_0; we denote the limit by $\hat{T}$.

We have shown that $F(\lambda - i\eta)$ has a tempered distribution $\hat{T}$ as a boundary value. It remains to prove that its inverse Fourier transform T has support in $\overline{\Gamma}_{a,\theta}$ and to verify (IX.14). Let $\eta_1 \in \Gamma^*_{a,\theta}$ be given and suppose that $\varphi \in C_0^\infty(\mathbb{R}^n)$ has compact support in the open half-space $\{x \mid \eta_1 \cdot x < 0\}$. Then there is $\varepsilon > 0$ so that $x \in$ supp φ implies $\eta_1 \cdot x \leq -\varepsilon$.

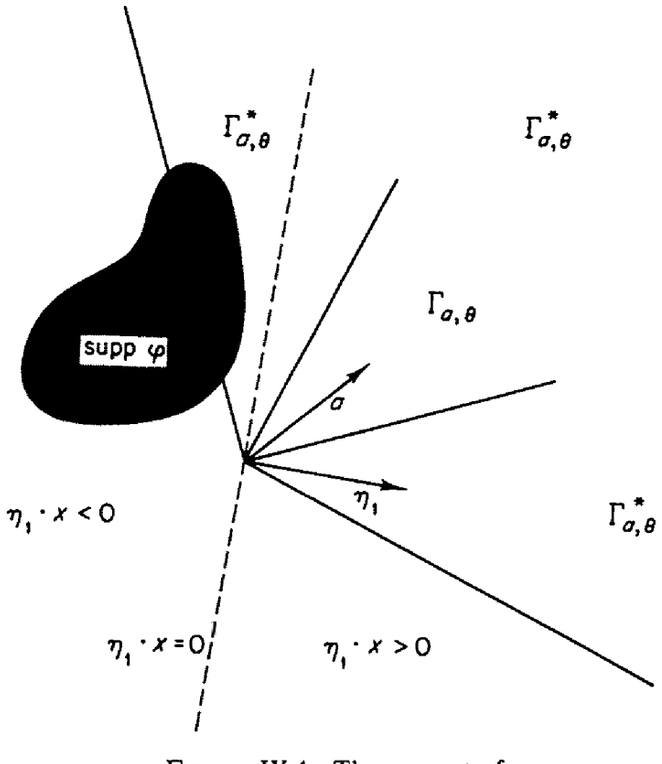


FIGURE IX.4 The support of φ.

See Figure IX.4. It follows that $\check{\varphi}$ is entire and that for each N

$$|\check{\varphi}(\lambda - is\eta_1)| = |(2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{i(\lambda - is\eta_1)\cdot x} \varphi(x)\, dx|$$

$$\leq \frac{C_N e^{-s\varepsilon}}{(1 + |\lambda - is\eta_1|^N)} \tag{IX.16}$$

for some constant C_N. Furthermore,

$$T_{t,\eta_1}(\varphi) = \hat{T}_{t,\eta_1}(\check{\varphi})$$

$$= \int F(\lambda - it\eta_1)\check{\varphi}(\lambda)\, d\lambda$$

$$= \int F(\lambda - i(t+s)\eta_1)\check{\varphi}(\lambda - is\eta_1)\, d\lambda$$

by Cauchy's formula. Thus, if we use the hypothesis (i) and choose N large enough in the estimate (IX.16), we find that for arbitrary $s > 0$,

$$|T_{t,\eta_1}(\varphi)| \leq Ce^{-s\varepsilon}$$

and thus $T_{t,\eta_1}(\varphi) = 0$. Therefore, the support of T_{t,η_1} is contained in the half-space $\{x \mid \eta_1 \cdot x \geq 0\}$ for each $t > 0$. Since $T_{t,\eta_1} \to T$ as $t \downarrow 0$, we conclude that supp $T \subset \{x \mid \eta_1 \cdot x \geq 0\}$. Since $\Gamma_{a,\theta}$ is the intersection of the closed subspaces $\{x \mid \eta_1 \cdot x \geq 0\}$ where η_1 runs through $\Gamma^*_{a,\theta}$, we see that supp $T \subset \Gamma_{a,\theta}$.

Finally, suppose $\check{\psi} \in C_0^\infty(\mathbb{R}^n)$ as above. Then

$$\int_{\mathbb{R}^n} F(\lambda - i\eta)\psi(\lambda)\, d\lambda = \int F(\tau - is\eta)\psi(\tau - (s-1)i\eta)\, d\tau$$

$$= \hat{T}_{s,\eta}(\widehat{e^{-(s-1)\eta\cdot x}\check{\psi}})$$

$$\xrightarrow[s\to 0]{} \hat{T}(\widehat{e^{\eta\cdot x}\check{\psi}})$$

$$= T(e^{-\eta\cdot x}\hat{\psi})$$

$$= (e^{-\eta\cdot x}T)(\hat{\psi})$$

$$= (\widehat{e^{-\eta\cdot x}T})(\psi)$$

This proves (IX.4) and completes the proof of the theorem. ∎

We will use this theorem in our study of axiomatic quantum field theory in Section 9.

IX.4 L^p Estimates

There are a large number of L^p-estimates on Fourier transforms and convolutions. These estimates are useful because they give conditions on p and q so that the Fourier transform or convolution by a given function is a bounded map from L^p to L^q. The proofs of the estimates typically require delicate use of L^p-interpolation theorems. In this section we state several L^p-interpolation theorems and give examples to show how they may be used to derive estimates. In the Appendix, we prove the first of these theorems (Theorem IX.17) and use the idea of this proof to prove a variety of other interpolation theorems not used in this section.

The simplest L^p-interpolation theorem is:

Theorem IX.17 (The Riesz–Thorin theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be measure spaces with σ-finite measures. Let $1 \leq p_0, p_1, q_0, q_1 \leq \infty$ and suppose that T is a linear transformation from $L^{p_0}(M, d\mu) \cap L^{p_1}(M, d\mu)$ to

$L^{q_0}(N, dv) \cap L^{q_1}(N, dv)$ which satisfies $\|Tf\|_{q_0} \le M_0\|f\|_{p_0}$ and $\|Tf\|_{q_1} \le M_1\|f\|_{p_1}$. Then, for each $f \in L^{p_0} \cap L^{p_1}$, and each $t \in (0, 1)$, $Tf \in L^{q_t}$ and $\|Tf\|_{q_t} \le C_t\|f\|_{p_t}$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$, $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$, and $C_t = M_0^{1-t}M_1^t$.

Notice that if the hypotheses of the theorem are satisfied, then T can be extended by the B.L.T. theorem to be a bounded map from $L^{p_t}(M, d\mu)$ to $L^{q_t}(N, dv)$. The Riesz–Thorin theorem says essentially that the set of $\langle p^{-1}, q^{-1}\rangle$ so that T: $L^p(M, d\mu) \to L^q(N, dv)$ is bounded is a convex subset of the plane and that on that subset the logarithm of the norm of T is a convex function. The Riesz–Thorin theorem is a special case of the Stein interpolation theorem which is proven in the Appendix at the end of this section.

We have already given one application of this theorem in Section 2 (the Hausdorff–Young theorem). Here is another:

Example 1 (Young's theorem and inequality) When f and g are in $\mathcal{S}(\mathbb{R}^n)$ we defined the convolution by the formula

$$(f * g)(x) = \int f(x-y)g(y)\,dy \tag{IX.17}$$

Suppose $p^{-1} + q^{-1} = 1$. If $f \in L^p(\mathbb{R}^n)$ and $g \in L^q(\mathbb{R}^n)$, then the integral converges absolutely for all x by Hölder's inequality. Thus we can use (IX.17) to define $f * g$ when $f \in L^p$, $g \in L^q$. Note that $\|f * g\|_\infty \le \|f\|_p\|g\|_q$. Next, suppose that $f, g \in L^1(\mathbb{R}^n)$. Then

$$\iint |f(x-y)g(y)|\,dx\,dy = \|f\|_1\|g\|_1$$

so by Fubini's theorem the integral in (IX.17) exists a.e. in x, and the function $f * g$ (defined a.e.) satisfies $\|f * g\|_1 \le \|f\|_1\|g\|_1$. We can now use the Riesz–Thorin theorem to define the convolution on other L^p spaces.

Suppose that $f \in L^1(\mathbb{R}^n)$. Then $T_f(g) = f * g$ is a bounded operator from $L^1(\mathbb{R}^n)$ to $L^1(\mathbb{R}^n)$ (of norm less than or equal to $\|f\|_1$) and from $L^\infty(\mathbb{R}^n)$ to $L^\infty(\mathbb{R}^n)$ (of norm less than or equal to $\|f\|_1$). Therefore, by the Riesz–Thorin theorem, T_f: $L^p(\mathbb{R}^n) \to L^p(\mathbb{R}^n)$ and has norm less than or equal to $\|f\|_1$. Now fix $g \in L^p(\mathbb{R}^n)$. Then

$$T_g\colon L^1(\mathbb{R}^n) \to L^p(\mathbb{R}^n), \qquad \|T_g\| \le \|g\|_p$$
$$T_g\colon L^q(\mathbb{R}^n) \to L^\infty(\mathbb{R}^n), \qquad \|T_g\| \le \|g\|_p$$

We now use the Riesz–Thorin theorem again to interpolate between 1 and q concluding that T_g: $L^r(\mathbb{R}^n) \to L^s(\mathbb{R}^n)$ with norm less than or equal to $\|g\|_p$ where $r^{-1} = 1 - tp^{-1}$ and $s^{-1} = (1-t)p^{-1}$. Eliminating t, we find that for $1 \le p, r, s, \le \infty$, satisfying $p^{-1} + r^{-1} = 1 + s^{-1}$,

$$\|f * g\|_s \le \|f\|_r\|g\|_p$$

This is known as Young's inequality.

It is sometimes important to know that the extended convolution from $L^p \times L^r$ to L^s which we have just defined by using the Riesz–Thorin theorem can still be computed a.e. by the integral formula (IX.17). The proof, like the extension, is in two stages. Let $p^{-1} + q^{-1} = 1$ and suppose that $f \in L^p$, $g \in L^1$, and $h \in L^q$. We may assume without loss that f, g, and h are positive. Then

$$\begin{aligned}\int h(x)\left(\int f(x-y)g(y)\,dy\right)dx &= \int g(y)\left(\int f(x-y)h(x)\,dx\right)dy\\ &\le \|f\|_p\|h\|_q\int g(y)\,dy\\ &= \|f\|_p\|h\|_q\|g\|_1\end{aligned}$$

Since this holds for all such h, the integral $\int f(x-y)g(y)\,dy$ converges a.e.[x] and is in L^p with norm less than or equal to $\|f\|_p\|g\|_1$. But the map $f \to \int f(x-y)g(y)\,dy$ agrees with the convolution for all $f \in L^1 \cap L^\infty$, so it agrees on all of L^p.

Now, we use the same trick again. Let $p^{-1} + r^{-1} = 1 + s^{-1}$ and suppose that $f \in L^p$, $g \in L^r$ and $h \in L^1 \cap L^{s'}$ where $s' = s(s-1)^{-1}$. Then, using the Hölder and Young inequalities we have

$$\begin{aligned}&\int g(y)\left(\int f(x-y)h(x)\,dx\right)dy\\ &\le \|g\|_r\|\tilde{f} * h\|_{r'}\\ &\le \|g\|_r\|\tilde{f}\|_p\|h\|_{s'}\end{aligned}$$

since by the first part of the argument the integral represents the convolution. Thus, by Fubini's theorem $g(y)f(x-y)h(x) \in L^1(\mathbb{R}^n \times \mathbb{R}^n)$, and as a function of y, $g(y)f(x-y)h(x) \in L^1(\mathbb{R}^n)$ for almost all x, and

$$\int h(x)\left(\int f(x-y)g(y)\,dy\right)dx \le \|g\|_r\|\tilde{f}\|_p\|h\|_{s'}$$

Since $h \in L^1 \cap L^{s'}$ was arbitrary, we conclude that $f(x-y)g(y) \in L^1(\mathbb{R}^n)$ as a function of y for almost all x and $\int f(x-y)g(y)\,dy \in L^s(\mathbb{R}^n)$ with norm less

than or equal to $\|f\|_p\|g\|_r$. Therefore, since the bounded maps $g \to f * g$ and $g \to \int f(x-y)g(y)\,dy$ agree on $L^1 \cap L^r$, they agree on L^r.

There is a classical result of Hardy and Littlewood which says that if $p^{-1} + q^{-1} + \lambda = 2$, $\lambda < 1$, and $p, q > 1$, then

$$\iint_{\mathbb{R}^2} |f(x)g(y)||x-y|^{-\lambda}\,dx\,dy < \infty \tag{IX.18}$$

if $f \in L^p(\mathbb{R})$, $g \in L^q(\mathbb{R})$. This is a strengthening of Young's inequality, since Young's inequality can easily be transformed into the statement that if $p^{-1} + r^{-1} + q^{-1} = 2$, then

$$\left| \iint_{\mathbb{R}^2} f(x)g(y)h(x-y)\,dx\,dy \right| < \infty$$

if $f \in L^p(\mathbb{R})$, $g \in L^r(\mathbb{R})$, $h \in L^q(\mathbb{R})$. (IX.18) is a strengthening of this inequality since $|x|^{-1} \notin L^1(\mathbb{R})$ and therefore $|x|^{-\lambda} \notin L^{\lambda^{-1}}(\mathbb{R})$. In order to deal with situations like this it is useful to introduce classes of functions which are barely not in the L^p spaces.

Definition Let $\langle M, \mu\rangle$ be a measure space, μ a σ-finite measure. A function f on M is said to be in **weak-L^p**, written $f \in L^p_w(M, d\mu)$, if there is a constant $C < \infty$ so that

$$\mu\{x \mid |f(x)| > t\} \le Ct^{-p} \qquad \text{for all } t > 0$$

If $f \in L^p_w$, we write

$$\|f\|_{p,w} = \sup_t (t^p \mu\{x \mid |f(x)| > t\})^{1/p}$$

Notice that $\|\cdot\|_{p,w}$ is not a norm since it does not satisfy the triangle inequality. The name weak-L^p comes from the fact that $L^p \subset L^p_w$ and $\|f\|_{p,w} \le \|f\|_p$ (see Problem 24). Further, $f \in L^p$ if and only if

$$\int_0^\infty \mu\{x \mid |f(x)| > t\} t^{p-1}\,dt < \infty$$

This integral is at worst logarithmically divergent if $f \in L^p_w$.

Example 2 The function $|x|^{-n/p}$ from $\mathbb{R}^n$ to $\mathbb{R}$ has $\mu\{x \mid |f(x)| > t\} = c_n t^{-p}$ where c_n is the volume of the unit ball in $\mathbb{R}^n$. Thus f is in $L^p_w(\mathbb{R}^n, dx)$ but f is not in $L^q(\mathbb{R}^n, dx)$ for any q.

We state without proof two interpolation theorems about weak-L^p spaces. The proof of Hunt's theorem is outlined in the problems. References are given in the notes.

Theorem IX.18 (Marcinkiewicz interpolation theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be σ-finite measure spaces and $1 \le p_0 \le q_0 \le \infty$, $1 \le p_1 \le q_1 \le \infty$, $q_0 \ne q_1$. Suppose that T is a linear transformation satisfying $T: L^{p_0}(M, d\mu) \to L^{q_0}_w(N, d\nu)$ and $T: L^{p_1}(M, d\mu) \to L^{q_1}_w(N, d\nu)$ with

$$\|T\varphi\|_{q_0,w} \le c_0\|\varphi\|_{p_0}$$
$$\|T\psi\|_{q_1,w} \le c_1\|\psi\|_{p_1}$$

for all $\varphi \in L^{p_0}(M, d\mu)$, $\psi \in L^{p_1}(M, d\mu)$. Then, for any $t \in (0, 1)$, T extends to a bounded linear transformation from $L^{p_t}(M, d\mu)$ to $L^{q_t}(N, d\nu)$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$ and $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$. The bound depends only on t and the c_i, q_i, and p_i.

Theorem IX.19 (Hunt's interpolation theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be σ-finite measure spaces and $1 \le p_1 < p_0 \le \infty$, $1 \le q_1 < q_0 \le \infty$. Suppose that T is a bounded linear transformation from $L^{p_0}(M, d\mu)$ to $L^{q_0}(N, d\nu)$ and from $L^{p_1}(M, d\mu)$ to $L^{q_1}(N, d\nu)$. Then for any $t \in (0, 1)$, T extends to a bounded linear map of $L^{p_t}_w(M, d\mu)$ to $L^{q_t}_w(N, d\nu)$ (p_t and q_t defined above). Moreover, $\|Tf\|_{q_t,w} \le C_t\|f\|_{p_t,w}$ where C_t depends only on t, p_i, q_i, and the bounds at the end points.

We remark that the Marcinkiewicz theorem is the deepest interpolation theorem since it turns "weak" information into strong information. The reader is cautioned to remember the $p < q$ condition (see Problem 77 for an example of the trouble that can be caused by forgetting it). Notice that we do not have the logarithmically convex bound in either of the "weak" theorems as we did in the Riesz–Thorin theorem.

As an application of how to use these theorems in tandem, we will prove a generalization of the Hardy–Littlewood inequality.

Example 3 (Sobolev's inequality) Let $0 < \lambda < n$ and suppose that $f \in L^p(\mathbb{R}^n)$, $h \in L^r(\mathbb{R}^n)$ with $p^{-1} + r^{-1} + \lambda n^{-1} = 2$ and $1 < p, r < \infty$. Then

$$\iint \frac{|f(x)||h(y)|}{|x-y|^\lambda}\,d^nx\,d^ny \le C_{p,r,\lambda,n}\|f\|_p\|h\|_r \tag{IX.19}$$

To prove this we need the following extension of Young's inequality: If $1 < p, r, s < \infty$, $p^{-1} + r^{-1} = s^{-1} + 1$, $f \in L^p(\mathbb{R}^n)$, $g \in L^r_w(\mathbb{R}^n)$, then

$f * g \in L^s(R^n)$ and $\|f * g\|_s \leq C\|f\|_p\|g\|_{r,w}$. First fix $f \in L^p(\mathbb{R}^n)$. Then Young's inequality (Example 1) shows that T_f: $L^r(\mathbb{R}^n) \to L^s(\mathbb{R}^n)$ where $T_f(g) = f * g$ and $1 \leq r \leq p'$. Choosing first $r = 1$ and then $r = p'$ and using Hunt's theorem we conclude that for $1 < r < p'$, T_f: $L^r_w(\mathbb{R}^n \to L^s_w(\mathbb{R}^n)$ is bounded. Now, we fix $g \in L^r_w(\mathbb{R}^n)$. We know that T_g: $L^p(\mathbb{R}^n) \to L^s_w(\mathbb{R}^n)$ is bounded for p and s suitably related and $p \leq s$. Using the Marcinkiewicz theorem we conclude that $f * g \in L^s(\mathbb{R}^n)$. Sobolev's inequality follows directly from this extended version of Young's inequality.

Table IX.1 summarizes some of the most important L^p inequalities on $\mathbb{R}^n$. There are also L^p estimates involving derivatives which we discuss in the Notes to Section IX.6.

TABLE IX.1

Name	Conditions	Inequality
Hölder	$1 \leq p, q, r \leq \infty$ $p^{-1} + q^{-1} = r^{-1}$	$\|fg\|_r \leq \|f\|_p\|g\|_q$
Hausdorff–Young	$1 \leq p \leq 2$ $p^{-1} + q^{-1} = 1$	$\|\hat{f}\|_q \leq (2\pi)^{(n/2-n/p)}\|f\|_p$
Young	$1 \leq p, q, r \leq \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_r \leq \|f\|_p\|g\|_q$
Generalized Young	$1 < p, q, r < \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_r \leq C_{p,q}\|f\|_p\|g\|_{q,w}$
Weak Hausdorff–Young	$1 < p < 2$ $p^{-1} + q^{-1} = 1$	$\|\hat{f}\|_{q,w} \leq C_{p,n}\|f\|_{p,w}$
Weak Young	$1 < r, p, s < \infty$ $p^{-1} + q^{-1} = 1 + r^{-1}$	$\|f * g\|_{r,w} \leq C_{p,q}\|f\|_{p,w}\|g\|_{q,w}$

Appendix to IX.4 Abstract interpolation

In this appendix, we prove an abstract interpolation theorem and then give several applications including a proof of the Stein and Riesz–Thorin theorems. Before turning to the abstract theory we present two propositions which illustrate the basic idea behind interpolation.

Proposition 1 Let A and B be matrices on the inner product space $\mathbb{C}^n$ with $A \geq 0$. Suppose that $\|AB\| \leq 1$ and $\|BA\| \leq 1$. Then $\|A^{1/2}BA^{1/2}\| \leq 1$.

Proof Suppose that Proposition 1 is true for all $A > 0$. Then we can prove the proposition for all $A \geq 0$ as follows. Given $A \geq 0$ and the conditions $\|AB\| \leq 1$, $\|BA\| \leq 1$, let $c > 0$ and define $B' = B(1 + c\|B\|)^{-1}$. Then $\|(A + c)B'\| \leq 1$ and $\|B'(A + c)\| \leq 1$. Since $A + c > 0$ we conclude that $\|(A + c)^{1/2}B'(A + c)^{1/2}\| \leq 1$. Letting $c \downarrow 0$ we conclude that

$$\|A^{1/2}BA^{1/2}\| \leq 1$$

Thus we may assume that $A > 0$.

How shall we turn information about AB and BA into information about $A^{1/2}BA^{1/2}$? Since A^x is a well-defined self-adjoint operator, it is natural to introduce the function $F(x) = A^xBA^{1-x}$. We then notice that $F(x)$ has an analytic continuation, $F(z) = A^zBA^{1-z} = e^{z \log A}Be^{(1-z)\log A}$ to the entire complex plane. Thus, the hypotheses of Proposition 1 tell us that the particular matrix-valued analytic function $F(z)$ has the properties $\|F(0)\| \leq 1$ and $\|F(1)\| \leq 1$. We must use these inequalities to conclude that $\|F(\frac{1}{2})\| \leq 1$. To do this we use a classical result in function theory due to Hadamard:

Lemma (Hadamard's three line theorem) Let $\varphi(z)$ be a complex-valued function, bounded and continuous on the closed strip $\{z \mid 0 \leq \operatorname{Re} z \leq 1\}$, analytic in the interior, satisfying

$$|\varphi(z)| \leq M_0 \quad \text{if} \quad \operatorname{Re} z = 0$$

and

$$|\varphi(z)| \leq M_1 \quad \text{if} \quad \operatorname{Re} z = 1$$

Then $|\varphi(z)| \leq M_0^{1-\operatorname{Re} z}M_1^{\operatorname{Re} z}$ for all z in the strip.

Proof We may take $M_0 = 1 = M_1$ since we can always replace $\varphi(z)$ by $\varphi(z)M_0^{z-1}M_1^{-z}$. We must show that $|\varphi(z)| \leq 1$ in the strip. If $\varphi(z) \to 0$ at ∞ in the strip, then $|\varphi(z)| \leq 1$ by the maximum modulus principle. Otherwise, consider $\varphi_n(z) = \varphi(z)e^{z^2/n}e^{-1/n}$. Since $\varphi(z)$ is bounded, $\varphi_n(z) \to 0$ as $z \to \infty$ in the strip. Thus, $|\varphi_n(z)| \leq 1$ everywhere in the strip since $|\varphi_n| \leq 1$ on the boundary. This is true for all n, so $|\varphi(z)| \leq 1$ since $e^{z^2/n}e^{-1/n} \to 1$ as $n \to \infty$. ∎

Hadamard's theorem holds for Banach space-valued analytic functions by the same proofs. We will use this extended theorem without comment. We can now easily prove Proposition 1.

Conclusion of the proof of Proposition 1 If $y \in \mathbb{R}$, then $e^{iy \log A}$ is unitary, so $\|e^{iy \log A}\| = 1$. Thus, on the line $\operatorname{Re} z = 0$, we have $\|F(z)\| = \|BA\| \leq 1$ and on the line $\operatorname{Re} z = 1$, we have $\|F(z)\| = \|AB\| \leq 1$. Moreover, for $0 \leq \operatorname{Re} z \leq 1$, $\|F(z)\| \leq (1 + \|A\|)^2 \|B\|$. Thus, by the three line theorem, $\|F(z)\| \leq 1$ for all z in the strip $0 \leq \operatorname{Re} z \leq 1$. In particular, $\|F(\frac{1}{2})\| \leq 1$. ∎

The reader is invited to find a proof of Proposition 1 which does not use interpolation (Problem 51). The three line theorem also gives an easy proof of Holder's inequality:

Proposition 2 (Hölder's inequality) Let $\langle M, \mu \rangle$ be a measure space and suppose that $f \in L^p(M, d\mu)$ and $g \in L^q(M, d\mu)$ where $p^{-1} + q^{-1} = 1$. Then $fg \in L^1(M, d\mu)$ and $\|fg\|_1 \leq \|f\|_p \|g\|_q$.

Proof It is sufficient to prove Hölder's inequality in the case where f and g are nonnegative simple functions (finite linear combinations of characteristic functions of disjoint measurable sets of finite measure). Let

$$F(z) = \int_M f^{pz} g^{q(1-z)} \, d\mu$$

Then $F(z)$ is continuous and bounded on the strip $0 \leq \operatorname{Re} z \leq 1$ and analytic in the interior. If $\operatorname{Re} z = 0$, then

$$|F(z)| \leq \int |f^{pz} g^{q(1-z)}| \, d\mu = \int |g|^q \, d\mu = \|g\|_q^q$$

and if $\operatorname{Re} z = 1$,

$$|F(z)| \leq \int |f^{pz} g^{q(1-z)}| \, d\mu = \int |f|^p \, d\mu = \|f\|_p^p$$

Thus, by the three line theorem $|F(x)| \leq \|g\|_q^{q(1-x)} \|f\|_p^{px}$ for all $0 \leq x \leq 1$. In particular for $x = p^{-1}$ we conclude that

$$F\left(\frac{1}{p}\right) = \int_M fg \, d\mu \leq \|g\|_q \|f\|_p \text{ ∎}$$

The Hadamard theorem lies behind a general approach to interpolation theorems using complex methods (for other approaches, see the references in the Notes). Our discussion is divided into two parts. First we show that if X is a vector space with two norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ obeying a consistency condition, then it is possible to define a natural family of Banach spaces $\{X_t \mid 0 \leq t \leq 1\}$ which interpolate between X_0 and X_1, the completions of X in $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$. The abstract interpolation theorem

then follows easily; namely if $\{X_t\}$ interpolates between X_0 and X_1 and $\{Y_t\}$ interpolates between Y_0 and Y_1, then any map T which is in $\mathscr{L}(X_0, Y_0)$ and in $\mathscr{L}(X_1, Y_1)$ extends uniquely to a bounded map of X_t into Y_t for each t. In the second part we illustrate how the abstract theorem may be applied in specific cases. In particular, we will prove the Stein interpolation theorem, for which the Riesz–Thorin theorem is an immediate corollary, and several other interpolation theorems. The difficulty involved in the special cases is the concrete identification of the spaces $\{X_t\}$ and $\{Y_t\}$.

Definition Let X be a complex vector space. Two norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ on X are called **consistent** if any sequence $\{x_n\}$ that converges to zero in one norm and which is Cauchy in the other norm converges to zero in both norms. If $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent, we define

$$\|x\|_+ = \inf\{\|y\|^{(0)} + \|z\|^{(1)} \mid x = y + z\}$$

Proposition 3 Let $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ be consistent norms on a complex vector space X. Then:

(a) $\|\cdot\|_+$ is a norm.

(b) If X_0, X_1, and X_+ denote the completions of X under $\|\cdot\|^{(0)}$, $\|\cdot\|^{(1)}$, and $\|\cdot\|_+$, then the identity map on X extends to a continuous *injective* map of X_0 into X_+ and of X_1 into X_+.

Proof Suppose that $x \in X$ and $\|x\|_+ = 0$. Then there exist y_n and z_n such that $x = y_n + z_n$ and $y_n \xrightarrow{\|\cdot\|^{(0)}} 0$, $z_n \xrightarrow{\|\cdot\|^{(1)}} 0$. But then $y_n = x - z_n \xrightarrow{\|\cdot\|^{(1)}} x$, so $x = 0$ by the consistency of the norms. This proves (a).

Since $\|\cdot\|_+ \leq \|\cdot\|^{(0)}$, the identity map $\imath$ extends uniquely to a continuous map of X_0 into X_+. Suppose that $x \in X_0$ and $\imath(x) = 0$. Then, there exist $x_n \in X$ such that $x_n \xrightarrow{\|\cdot\|^{(0)}} x$ and $x_n \xrightarrow{\|\cdot\|_+} 0$. The second statement implies that there exist y_n, $z_n \in X$ so that $x_n = y_n + z_n$, $y_n \xrightarrow{\|\cdot\|^{(0)}} 0$, and $z_n \xrightarrow{\|\cdot\|^{(1)}} 0$. Thus, $z_n = x_n - y_n \xrightarrow{\|\cdot\|^{(0)}} x$. Since $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent, $z_n \xrightarrow{\|\cdot\|^{(0)}} 0$, so $\imath: X_0 \to X_+$ is injective. The proof for X_1 is the same. ∎

The converse of this proposition is also true: namely, if $\|\cdot\|_+$ is a norm and the extensions of $\imath$ are injective, then $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ are consistent. The reader can familiarize himself with consistent and nonconsistent norms by doing Problem 34. **The space $X_0 \cap X_1$ may be strictly larger than X, but if we replace X by this larger space and repeat the above construction, we obtain the same X_0, X_1, etc. We henceforth suppose without loss that $X = X_0 \cap X_1$.**

Let S denote the closed strip $\{z \in \mathbb{C} \mid 0 \le \operatorname{Re} z \le 1\}$, S° the interior of S, and let $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$ be two consistent norms on a complex vector space X. We define $\mathscr{F}(X)$ to be the set of continuous functions f from S to X_+ which are analytic in S° and which satisfy:

(i) if $\operatorname{Re} z = 0$, then $f(z) \in X_0$ and $t \to f(it)$ is continuous in $\|\cdot\|^{(0)}$; if $\operatorname{Re} z = 1$, then $f(z) \in X_1$ and $t \to f(1 + it)$ is continuous in $\|\cdot\|^{(1)}$.

(ii) $\sup_{z \in S} \|f(z)\|_+ < \infty$;

(iii) $|||f||| \equiv \sup_{t \in \mathbb{R}} \{\|f(it)\|^{(0)}, \|f(1 + it)\|^{(1)}\} < \infty$.

Proposition 4

(a) $\mathscr{F}(X)$ with the norm $|||\cdot|||$ is a Banach space.

(b) For each $t \in [0, 1]$, the subspace

$$K_t = \{f \in \mathscr{F}(X) \mid f(t) = 0\}$$

is $|||\cdot|||$-closed.

Proof $|||\cdot|||$ is clearly positive, subadditive, and positive homogeneous. By the three line theorem and the estimates $\|\cdot\|_+ \le \|\cdot\|^{(i)}$, $i = 0, 1$, we see that

$$\sup_{z \in S} \|f(z)\|_+ \le \sup_{\operatorname{Re} z = 0, 1} \|f(z)\|_+ \le |||f||| \tag{IX.20}$$

Thus $|||f||| = 0$ implies that $f \equiv 0$, so $|||\cdot|||$ is a norm on $\mathscr{F}(X)$. To see that $\mathscr{F}(X)$ is complete, let $\{f_n\}$ be a Cauchy sequence in $\mathscr{F}(X)$. By (IX.20), the functions converge uniformly to a bounded continuous function f on S. By the uniform convergence, f is analytic in S° and satisfies properties (i), (ii), and (iii). This completeness argument also shows that each of the subspaces K_t is closed. ∎

We now define

$$\tilde{X}_t = \mathscr{F}(X)/K_t, \qquad 0 \le t \le 1$$

We will denote the quotient norm on $\tilde{X}_t$ by $\|\cdot\|^{(t)}$. Notice that X may be identified with a subset of $\tilde{X}_t$ under the map which takes each $x \in X$ into $[x]$, the equivalence class of the constant function whose value is x. Further, $\tilde{X}_t$ may be identified with a subset of X_+ under the map which takes an equivalence class $[f]$ into the common value of its members at t. This map is clearly injective and the following computation shows that it is continuous: Let $[f] \in \tilde{X}_t$ and $x = f(t)$. By (IX.20), $\|x\|_+ \le |||f|||$. Thus

$$\|x\|_+ \le \inf\{|||f||| \mid f \in \mathscr{F}(X), f(t) = x\} = \|[f]\|^{(t)}$$

We now define X_t to be the completion of X in the norm $\|\cdot\|^{(t)}$. Thus, the spaces we have defined are related as follows:

$$X \to X_t \to \tilde{X}_t \to X_+$$

where each $\to$ is a continuous injective map. For $t = 0$ (respectively, $t = 1$), X_t is just the space X_0 (respectively, X_1) which we started with. To see this, let $x \in X$ and let $\|\cdot\|^{(0)}$ denote the original zero norm. If $f \in \mathscr{F}(X)$ and $f(0) = x$, then

$$\|x\|^{(0)} \le \sup_{y \in \mathbb{R}} \{\|f(iy)\|^{(0)}, \|f(1 + iy)\|^{(1)}\} = |||f|||$$

so,

$$\|x\|^{(0)} \le \inf\{|||f||| \mid f(0) = x\}$$

Conversely, let $c > 0$ and consider $f_c(z) = e^{-cz}x$. Then, $\|f_c(iy)\|^{(0)} = \|x\|^{(0)}$ and $\sup_{y \in \mathbb{R}} \|f_c(1 + iy)\|^{(1)}$ can be made arbitrarily small by choosing c large. Thus

$$\|x\|^{(0)} = \inf\{|||f||| \mid f(0) = x\}$$

i.e., the quotient norm is just the norm $\|\cdot\|^{(0)}$ previously defined. The proof for $t = 1$ is the same. The spaces X_t are called **interpolation spaces** between X_0 and X_1 and the norms $\|\cdot\|^{(t)}$ are called **interpolating norms** between $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$.

We remark that it is possible (though not easy, see Problem 37) to prove that $X_t = \tilde{X}_t$, but we will not need this fact. We need to know only that the norm on X_t is equal (by definition) to the quotient norm on $\mathscr{F}(X)/K_t$. Later in the examples when we will have to identify X_t with a given Banach space B_t, we will always do this by showing that both X_t and B_t are the completions of X in the same norm.

Theorem IX.20 (Calderón–Lions interpolation theorem) Let X and Y be complex vector spaces with given consistent norms $\|\cdot\|_X^{(0)}$ and $\|\cdot\|_X^{(1)}$ on X and $\|\cdot\|_Y^{(0)}$ and $\|\cdot\|_Y^{(1)}$ on Y. Suppose that $T(\cdot)$ is an analytic, uniformly bounded, continuous, $\mathscr{L}(X_+, Y_+)$-valued function on the strip S with the following properties:

(i) $T(t)\colon X \to Y$ for each $t \in (0, 1)$

(ii) For all $y \in \mathbb{R}$, $T(iy) \in \mathscr{L}(X_0, Y_0)$ and

$$M_0 = \sup_{y \in \mathbb{R}} \|T(iy)\|_{\mathscr{L}(X_0, Y_0)} < \infty$$

(iii) For all $y \in \mathbb{R}$, $T(1+iy) \in \mathscr{L}(X_1, Y_1)$ and

$$M_1 = \sup_{y \in \mathbb{R}} \|T(1+iy)\|_{\mathscr{L}(X_1, Y_1)} < \infty$$

Then for any $t \in (0, 1)$,

$$T(t)[X_t] \subset Y_t$$

and

$$\|T(t)\|_{\mathscr{L}(X_t, Y_t)} \leq M_0^{1-t} M_1^t$$

Proof Let $U(z) = M_0^{z-1} M_1^{-z} T(z)$. Then $U(\cdot)$ obeys the same properties as $T(\cdot)$ except that the bounds on $U(z)$ when $\operatorname{Re} z = 0$ and $\operatorname{Re} z = 1$ are equal to one. Thus, without loss of generality we may assume that $M_0 = M_1 = 1$.

If $f \in \mathscr{F}(X)$, then $T(z)f(z)$ is a continuous, bounded Y_+-valued function on S, analytic on S°. By hypotheses (ii) and (iii),

$$\|T(iy)f(iy)\|_Y^{(0)} \leq \|f(iy)\|_X^{(0)}$$
$$\|T(1+iy)f(1+iy)\|_Y^{(1)} \leq \|f(1+iy)\|_X^{(1)}$$

for each $y \in \mathbb{R}$. Thus, the map $J: \mathscr{F}(X) \to \mathscr{F}(Y)$ given by $(Jf)(z) = T(z)f(z)$ has norm less than or equal to one. Furthermore, if

$$K_t^X = \{f \in \mathscr{F}(X) \mid f(t) = 0\} \qquad \text{and} \qquad K_t^Y = \{f \in \mathscr{F}(Y) \mid f(t) = 0\},$$

then $J[K_t^X] \subset K_t^Y$. Thus, J lifts to a contraction $\tilde{J}_t: \tilde{X}_t \to \tilde{Y}_t$. Since $\tilde{J}_t$ acts on equivalence classes by $\tilde{J}_t[f] = [T(t)f(t)]$, we see that $\tilde{J}_t$ equals $T(t) \restriction \tilde{X}_t$ under the natural identification of $\tilde{X}_t$ with a subset of X_+. Finally, since $T(t): X \to Y$, $T(t)[X_t] \subset Y_t$. ∎

We now present several examples which show how to apply this abstract interpolation theorem.

Example 1 (L^p spaces) Let $\langle M, \mu \rangle$ be a σ-finite measure space and suppose $1 \leq p_0 < p_1 \leq \infty$. Let $X = L^{p_0}(M, d\mu) \cap L^{p_1}(M, d\mu)$ and let $\|\cdot\|^{(0)} = \|\cdot\|_{p_0}$, $\|\cdot\|^{(1)} = \|\cdot\|_{p_1}$. We will show that $X_t = L^{p_t}(M, d\mu)$, $0 \leq t \leq 1$, where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$, except when $p_1 = \infty$ in which case at $t = 1$, X_1 is the closure of X in the $\|\cdot\|_\infty$-norm (which may be smaller than $L^\infty(M, d\mu)$). The proof consists in showing that the $\|\cdot\|^{(t)}$-norm and the $\|\cdot\|_{p_t}$-norm agree on the simple functions which are dense in X. Let $t \in (0, 1)$ and let $\varphi(x)$ be a simple function with $\|\varphi\|_{p_t} = 1$ and define

$$f(z) = |\varphi(\cdot)|^{p_t(zp_1^{-1} + (1-z)p_0^{-1})} \exp(i \arg \varphi(\cdot))$$

Then for each $z \in S$, $f(z) \in X$, and

$$\|f(iy)\|_{L^{p_0}(M, d\mu)}^{p_0} = \int_M \left| |\varphi(x)|^{p_t p_0 (iyp_1^{-1} + (1-iy)p_0^{-1})} \right| d\mu(x)$$
$$= \int_M |\varphi(x)|^{p_t} \, d\mu(x) = 1$$

If $p_1 = \infty$, $\|f(1+iy)\|_\infty = 1$ and if $p_1 < \infty$, then

$$\|f(1+iy)\|_{L^{p_1}(M, d\mu)}^{p_1} = \int_M \left| |\varphi(x)|^{p_t p_1 ((1+iy)p_1^{-1} - iyp_0^{-1})} \right| d\mu(x)$$
$$= \int_M |\varphi(x)|^{p_t} \, d\mu(x) = 1$$

Therefore, $|||f||| = 1$, so $\|f(t)\|^{(t)} = \|f\|_{\mathscr{F}(X)/K_t} \leq 1$. Since the value of f at t is φ, we have $\|\varphi\|^{(t)} \leq 1$. Thus, we have shown that $\|\varphi\|^{(t)} \leq \|\varphi\|_{L^{p_t}}$ for all simple functions φ.

To prove the converse inequality, let $f \in \mathscr{F}(X)$ and let φ be a simple function on M. Let

$$g(z) = |\varphi(\cdot)|^{q_t(zq_1^{-1} + (1-z)q_0^{-1})} \exp(i \arg \varphi(\cdot))$$

where $q_t^{-1} = 1 - p_t^{-1}$. Then, since $f(z)$ is analytic and bounded as an X_+-valued function, $H(z) = \int_M f(z)g(z) \, d\mu$ is analytic and bounded in S and $H(t) = \int \varphi f(t) \, d\mu$. By the three line theorem,

$$\begin{aligned}
|H(t)| &\leq \sup_{y \in \mathbb{R}} \{|H(iy)|, |H(1+iy)|\} \\
&\leq \sup\{\|f(iy)g(iy)\|_{L^1}, \|f(1+iy)g(1+iy)\|_{L^1}\} \\
&\leq \sup_{y \in \mathbb{R}} \{\|f(iy)\|_{L^{p_0}} \|g(iy)\|_{L^{q_0}}, \|f(1+iy)\|_{L^{p_1}} \|g(1+iy)\|_{L^{q_1}}\} \\
&\leq (\sup\{\|f(iy)\|_{L^{p_0}}, \|f(1+iy)\|_{L^{p_1}}\})(\sup\{\|g(iy)\|_{L^{q_0}}, \|g(1+iy)\|_{L^{q_1}}\}) \\
&= |||f||| \cdot |||g||| \\
&= \|\phi\|_{q_t} |||f|||
\end{aligned}$$

by the above computation. Note that the above triple norms are different: one is obtained from L^{p_0} and L^{p_1}, the second from L^{q_0} to L^{q_1}. Since

$$\left| \int \varphi f(t) \, d\mu \right| \leq \|\varphi\|_{q_t} |||f|||$$

we conclude that $f \in L^{p_t}$ and

$$\|f(t)\|_{L^{p_t}} \leq |||f|||$$

It follows that for ψ simple and $f \in \psi + K_t$:

$$\|\psi\|^{(t)} = \inf_{f \in \psi + K_t} |||f|||$$
$$\geq \|\psi\|_{L^{p_t}}$$

Thus the norms $\|\cdot\|_{p_t}$ and $\|\cdot\|^{(t)}$ agree on simple functions. Since $X = L^{p_0} \cap L^{p_1}$ and the simple functions are dense in X_t and L^{p_t}, we conclude that $X_t = L^{p_t}$.

Combining the fact we have proven, namely $L^{p_t} = X_t$, with the abstract interpolation theorem we obtain:

Theorem IX.21 (the Stein interpolation theorem) Let $\langle M, \mu\rangle$ and $\langle N, \nu\rangle$ be σ-finite measure spaces and $1 \leq p_0, p_1, q_0, q_1 \leq \infty$. Suppose that $T(\cdot)$ is a continuous $\mathscr{L}(L^{p_0}(M, d\mu) + L^{p_1}(M, d\mu), L^{q_0}(N, d\nu) + L^{q_1}(N, d\nu))$-valued function on the strip $S = \{z \mid 0 \leq \operatorname{Re} z \leq 1\}$ which is uniformly bounded, analytic in the interior, and which satisfies

(i) $T(z)$: $L^{p_0} \cap L^{p_1} \to L^{q_0} \cap L^{q_1}$ for all $z \in S$.

(ii) For all $y \in \mathbb{R}$, $T(iy) \in \mathscr{L}(L^{p_0}(M, d\mu), L^{q_0}(N, d\nu))$ and

$$M_0 = \sup_{y \in \mathbb{R}} \|T(iy)\|_{\mathscr{L}(L^{p_0}, L^{q_0})} < \infty$$

(iii) For all $y \in \mathbb{R}$, $T(1 + iy) \in \mathscr{L}(L^{p_1}(M, d\mu), L^{q_1}(N, d\nu))$ and

$$M_1 = \sup_{y \in \mathbb{R}} \|T(1 + iy)\|_{\mathscr{L}(L^{p_1}, L^{q_1})} < \infty$$

Then for each $t \in (0, 1)$

$$T(t): L^{p_t}(M, d\mu) \to L^{q_t}(N, d\nu)$$

and

$$\|T(t)\|_{\mathscr{L}(L^{p_t}, L^{q_t})} \leq M_0^{1-t} M_1^t$$

where $p_t^{-1} = tp_1^{-1} + (1 - t)p_0^{-1}$, $q_t^{-1} = tq_1^{-1} + (1 - t)q_0^{-1}$.

Using the fact that $\tilde{X}_t = X$ it is possible to remove condition (i) from both the Stein and Calderón–Lions theorems. We also remark that the conclusion of the theorem still holds if only the weaker analyticity assumption, that $\int_N (T(z)\varphi)(y)\psi(y)\, d\nu(y)$ is analytic for all simple functions φ and ψ, is assumed to hold. The Riesz–Thorin theorem is an immediate corollary of the Stein interpolation theorem for we just take $T(z) = T$ for all z.

Example 2 ($\mathscr{I}_p$) Let $\mathscr{H}$ be a separable Hilbert space. Recall that the trace class $\mathscr{I}_1$ is the set of $A \in \mathscr{L}(\mathscr{H})$ so that $\operatorname{tr}(|A|) < \infty$ and that $\mathscr{I}_1$ is the dual of the compact operators $\operatorname{Com}(\mathscr{H})$ (Theorem VI.26). For $1 \leq p < \infty$, we define

$$\mathscr{I}_p = \{A \in \mathscr{L}(\mathscr{H}) \mid |A|^p \in \mathscr{I}_1\}$$

and set $\|A\|_p = (\operatorname{tr}(|A|^p))^{1/p}$. For $p = \infty$, we set $\mathscr{I}_\infty = \operatorname{Com}(\mathscr{H})$ with $\|A\|_\infty = \|A\|$. If $|A|^p \in \mathscr{I}_1$, then by the Riesz–Schauder theorem (Theorem VI.15) $\sigma(|A|^p)\backslash\{0\}$ consists of isolated eigenvalues of finite multiplicity. It follows that $|A|$ is compact so $A = U|A|$ is compact since $\operatorname{Com}(\mathscr{H})$ is an ideal of $\mathscr{L}(\mathscr{H})$. By Theorem VI.17, A may be represented as $A = \sum_{n=1}^N \lambda_n(\psi_n, \cdot)\varphi_n$ where $\{\psi_n\}$ and $\{\varphi_n\}$ are orthonormal sets and the λ_n are the singular values of A (nonzero eigenvalues of $|A|$). Thus,

$$|A| = \sum_{n=1}^N \lambda_n(\psi_n, \cdot)\psi_n \qquad \text{and} \qquad |A|^p = \sum_{n=1}^N \lambda_n^p(\psi_n, \cdot)\psi_n$$

so

$$\|A\|_p = (\operatorname{tr}(|A|^p))^{1/p} = \left(\sum_{n=1}^N \lambda_n^p\right)^{1/p}$$

That is, $\mathscr{I}_p$ is just the set of compact operators whose singular values are in ℓ_p and the norms are equal. This remains true even if $p = \infty$.

Proposition 5 Let $1 \leq p \leq \infty$ and $q^{-1} + p^{-1} = 1$. If $A \in \mathscr{I}_p$ and $B \in \mathscr{I}_q$, then $AB \in \mathscr{I}_1$ and $\|AB\|_1 \leq \|A\|_p \|B\|_q$.

Proof For $p = 1$, $q = \infty$, this is just Problem 28 of Chapter VI. For $1 < p < \infty$, the proof is similar to the proof of the Hölder inequality given in Proposition 2: Let $A = U|A|$ and $B = V|B|$ be the polar decompositions of A and B and define

$$F(z) = \operatorname{tr}(U|A|^{pz}V|B|^{q(1-z)})$$

$F(z)$ is bounded and continuous on the strip $S = \{z \mid 0 \leq \operatorname{Re} z \leq 1\}$ and analytic in the interior. Since $|A|^{pz}$ is unitary on the line $\operatorname{Re} z = 0$ and $|B|^{q(1-z)}$ is unitary on the line $\operatorname{Re} z = 1$,

$$\begin{aligned} |F(iy)| &= |\operatorname{tr}(U|A|^{iyp}V|B|^q|B|^{iyq})| \\ &\leq \operatorname{tr}(|B|^q) = \|B\|_q^q \\ |F(1 + iy)| &= |\operatorname{tr}(U|A|^p|A|^{iyp}V|B|^{-iyq})| \\ &\leq \operatorname{tr}(|A|^p) = \|A\|_p^p \end{aligned}$$

We have used the properties of the trace that $\operatorname{tr}(CD) = \operatorname{tr}(DC)$ and $|\operatorname{tr}(CD)| \le \|D\| \operatorname{tr}(C)$ if $C \ge 0$. Thus, by the three line theorem $|F(z)| \le \|A\|_p^{pz} \|B\|_q^{q(1-z)}$ for all z in $(0, 1)$. In particular, for $z = p^{-1}$, we find

$$|\operatorname{tr}(AB)| = \left| F\left(\frac{1}{p}\right) \right| \le \|A\|_p \|B\|_q \quad \blacksquare$$

Suppose that $A = U|A| \in \mathscr{I}_p$ and define $B = |A|^{p-1} U^* \|A\|_p^{-p/q}$. Then

$$\begin{aligned} \|B\|_q &= \operatorname{tr}[\,||A|^{p-1}U^*|^q]^{1/q} \|A\|_p^{-p/q} \\ &= \operatorname{tr}[(U|A|^{2(p-1)}U^*)^{q/2}]^{1/q} \|A\|_p^{-p/q} \\ &= \operatorname{tr}[U|A|^{q(p-1)}U^*]^{1/q} \|A\|_p^{-p/q} \\ &= \operatorname{tr}[\,|A|^{q(p-1)}]^{1/q} \|A\|_p^{-p/q} \\ &= 1 \end{aligned}$$

since $\operatorname{Ker} U = \operatorname{Ker} A$. A similar computation shows that $\operatorname{tr}(AB) = \|A\|_p$. Thus, by Proposition 5,

$$\|A\|_p = \sup_{\|D\|_q = 1} |\operatorname{tr}(AD)|$$

Now, suppose that A and C are in $\mathscr{I}_p$. Then

$$\begin{aligned} \|A + C\|_p &= \sup_{\|D\|_q = 1} |\operatorname{tr}((A + C)D)| \\ &\le \sup_{\|D\|_q = 1} |\operatorname{tr}(AD)| + \sup_{\|D\|_q = 1} |\operatorname{tr}(CD)| \\ &= \|A\|_p + \|C\|_p \end{aligned}$$

Thus $\mathscr{I}_p$ is a vector space and $\|\cdot\|_p$ is a norm on $\mathscr{I}_p$.

Proposition 6 Let $1 \le p \le \infty$. Then

(a) $\mathscr{I}_p$ is a Banach space with norm $\|\cdot\|_p$.
(b) $\mathscr{I}_1 \subset \mathscr{I}_p \subset \operatorname{Com}(\mathscr{H})$ and $\mathscr{I}_p$ is the closure of the finite rank operators in the norm $\|\cdot\|_p$.
(c) If $A \in \mathscr{I}_p$, then $A^* \in \mathscr{I}_p$ and $\|A^*\|_p = \|A\|_p$.

Proof For $p = \infty$, (a), (b), and (c) are standard properties of the compact operators. So, suppose $1 \le p < \infty$. For any sequence $\{\lambda_n\}$,

$$\|\{\lambda_n\}\|_\infty \le \|\{\lambda_n\}\|_p \le \|\{\lambda_n\}\|_1$$

so

$$\|A\| \le \|A\|_p \le \|A\|_1$$

Thus any Cauchy sequence $\{A_n\}$ in $\mathscr{I}_p$ converges in the uniform norm to a limiting operator A. The reader can easily check for himself that $A \in \mathscr{I}_p$

and $\|A_n - A\|_p \to 0$. Therefore, $\mathscr{I}_p$ is complete in the norm $\|\cdot\|_p$. As indicated above, each $A \in \mathscr{I}_p$ is compact and $\|A\|_p = \|\{\lambda_n\}\|_{\ell_p}$ where the $\{\lambda_n\}$ are the singular values of A in the representation $A = \sum_{n=1}^{\infty} \lambda_n(\psi_n, \cdot)\varphi_n$. Thus, the finite rank operators $A_M = \sum_{n=1}^{M} \lambda_n(\psi_n, \cdot)\varphi_n$ converge to A in the $\|\cdot\|_p$-norm. The inclusions $\mathscr{I}_1 \subset \mathscr{I}_p \subset \operatorname{Com}(\mathscr{H})$ follow immediately from the above inequality. This proves (a) and (b).

To prove (c) we observe that A and A^* have the same singular values. $\blacksquare$

Proposition 7 If $1 < p, q < \infty$ and $p^{-1} + q^{-1} = 1$, then $\mathscr{I}_p^* = \mathscr{I}_q$.

Proof Proposition 5 and the remark thereafter show that for each $A \in \mathscr{I}_q$ the map $B \to \operatorname{tr}(AB)$ is a bounded linear functional on $\mathscr{I}_p$ of norm $\|A\|_q$. Conversely, let $\Lambda \in \mathscr{I}_p^*$. Then since $\|A\|_p \le \|A\|_1$, $\Lambda \in \mathscr{I}_1^*$ so by Theorem VI.26 there is an $A \in \mathscr{L}(\mathscr{H})$ so that $\Lambda(B) = \operatorname{tr}(AB)$ for all $B \in \mathscr{I}_1$. We want to show that $A \in \mathscr{I}_q$. A may be written $D + iC$ where D and C are self-adjoint. Since

$$|\operatorname{tr}(A^*B)| = |\operatorname{tr}(AB^*)| \le \|\Lambda\| \, \|B^*\|_p = \|\Lambda\| \, \|B\|_p$$

we have

$$|\operatorname{tr}(DB)| \le \|\Lambda\| \, \|B\|_p, \qquad |\operatorname{tr}(CB)| \le \|\Lambda\| \, \|B\|_p$$

Thus it is sufficient to prove that $A \in \mathscr{I}_q$ in the case where A is self-adjoint. Let $a > 0$ and $E(a, \infty)$ be the spectral projections of A corresponding to the interval (a, ∞). Suppose $E(a, \infty)$ is infinite dimensional and let $\{\varphi_n\}$ be an orthonormal basis for $E(a, \infty)$. If we define

$$B_M = \left(\sum_{n=1}^{M} \frac{1}{n} P_{\varphi_n} \right) \left(\sum_{n=1}^{M} \frac{1}{n^p} \right)^{-1/p}$$

where P_{φ_n} is the projection onto φ_n, we have $\|B_M\|_p = 1$. But

$$\operatorname{tr}(AB_M) \ge \left(\sum_{n=1}^{M} \frac{a}{n} \right) \left(\sum_{n=1}^{M} \frac{1}{n^p} \right)^{-1/p} \xrightarrow{M \to \infty} \infty$$

which contradicts the fact that $|\operatorname{tr}(AB_M)| \le \|\Lambda\|$. Thus, $E(a, \infty)$ is finite dimensional and a similar proof shows that $E(-\infty, -a)$ is finite dimensional. It follows that A is compact and therefore may be represented as $A = \sum_{n=1}^{\infty} \mu_n P_{\psi_n}$ for some orthonormal set $\{\psi_n\}$. If $\{\gamma_n\}_{n=1}^{M}$ is any finite sequence so that $(\sum_1^M |\gamma_n|^p)^{1/p} = 1$, then $B_\gamma = \sum_1^M \gamma_n P_{\psi_n} \in \mathscr{I}_p$ and

$$\left| \sum_1^M \gamma_n \mu_n \right| = |\operatorname{tr}(AB_\gamma)| \le \|\Lambda\|$$

so $\{\mu_n\} \in \ell_q$ since $\ell_q = \ell_p^*$. Thus, $(\operatorname{tr}(|A|^q))^{1/q} = (\sum |\mu_n|^q)^{1/q} < \infty$ and $A \in \mathscr{I}_q$. $\blacksquare$

Proposition 8 Let $1 \le p_0 < p_1 \le \infty$ and define $X = \mathscr{I}_{p_0}$. Then $\|\cdot\|^{(0)} = \|\cdot\|_{p_0}$ and $\|\cdot\|^{(1)} = \|\cdot\|_{p_1}$ are consistent norms on X and $X_t = \mathscr{I}_{p_t}$ where $p_t = tp_1^{-1} + (1-t)p_0^{-1}$.

We omit the proof of Proposition 8; it is almost identical to the proof in Example 1 except that the decomposition $\varphi(x) = |\varphi(x)| \exp(i \arg \varphi(x))$ is replaced by the decomposition $A = U|A|$ and the integral is replaced by the trace.

Theorem IX.22 Let $\mathscr{H}_1$ and $\mathscr{H}_2$ be separable Hilbert spaces with corresponding spaces $\mathscr{I}_p^{(1)}$, $\mathscr{I}_q^{(2)}$ of operators. Suppose that T takes $\mathscr{F}_1$, the finite rank operators on $\mathscr{H}_1$, into $\mathrm{Com}(\mathscr{H}_2)$, and that

(i) $\|T(A)\|_{q_0} \le M_0 \|A\|_{p_0}$ for all $A \in \mathscr{F}_1$.
(ii) $\|T(A)\|_{q_1} \le M_1 \|A\|_{p_1}$ for all $A \in \mathscr{F}_1$.

Then $\|T(A)\|_{q_t} \le M_1^t M_0^{1-t} \|A\|_{p_t}$ for all $A \in \mathscr{F}_1$ so T extends uniquely to a bounded map of $\mathscr{I}_{p_t}$ into $\mathscr{I}_{q_t}$ where $p_t^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$ and $q_t^{-1} = tq_1^{-1} + (1-t)q_0^{-1}$.

Proof The theorem follows immediately from Proposition 8 and the Calderón–Lions interpolation theorem. ∎

Example 3 (rigged Hilbert spaces) Let $\mathscr{H}$ be a Hilbert space and suppose that A is a positive self-adjoint operator on $\mathscr{H}$ with $\mathrm{Ker}\, A = \{0\}$ so that A^{-1} is also self-adjoint (both A and A^{-1} may be unbounded). Let $X = C^\infty(A) \cap C^\infty(A^{-1})$ and for each $m \in \mathbb{R}$, let $\mathscr{H}_m$ be the completion of X in the norm $\|\varphi\|_m = \|A^{m/2}\varphi\|_{\mathscr{H}}$. By the spectral theorem we may assume that $\mathscr{H} = L^2(M, d\mu)$ where $\langle M, \mu\rangle$ is a measure space and A is multiplication by a function $f \ge 0$. Clearly, $\mathscr{H}_m = L^2(M, f^m\, d\mu)$, and a short argument shows that the norms $\|\cdot\|_m$ are consistent. Let m_0 and m_1 be fixed, $m_t = tm_1 + (1-t)m_0$. Then a similar proof to that in Example 1 shows that $X_t = \mathscr{H}_{m_t}$. The proof that $\mathscr{H}_{m_t} \subset X_t$ uses the function $F(z) = f(\cdot)^{zm_1 + (1-z)m_0}$. The proof that $X_t \subset \mathscr{H}_{m_t}$ uses the natural identification of $\mathscr{H}_m^*$ with $\mathscr{H}_{-m}$. The reader is asked to provide the details in Problem 35. Once one has identified X_t as H_{m_t}, the abstract interpolation theorem can be applied to make concrete statements about operators on $\mathscr{H}$. Here are two simple examples:

Proposition 9 Let A and B be positive self-adjoint operators with (possibly unbounded) inverses on a Hilbert space $\mathscr{H}$. Let T be a bounded linear transformation of $\mathscr{H}$ into itself which satisfies:

(i) $\|T\varphi\| \le M_0\|\varphi\|$ for all $\varphi \in \mathscr{H}$.
(ii) $T: D(A^2) \to D(B^2)$ and $\|B^2 T\varphi\| \le M_1 \|A^2\varphi\|$ for all $\varphi \in D(A^2)$.

Then $T: D(A) \to D(B)$ and

$$\|BT\varphi\| \le M_0^{1/2} M_1^{1/2} \|A\varphi\| \qquad \text{for all } \varphi \in D(A)$$

Proposition 10 For $m \in \mathbb{R}$ let W_m be the mth Sobolev space (defined in Section IX.6). Suppose that $g \in C^k$ and $D^\alpha g$ is bounded for all α with $|\alpha| \le k$. Then, for each m with $|m| \le k$, $f \mapsto gf$ is a bounded map of W_m into W_m.

Proof We first show that $g: W_k \to W_k$ is bounded. By Proposition 1 of Section IX.6, $f \in W_k$ if and only if $D^\alpha f \in L^2$ for all $|\alpha| \le k$. From this it follows easily that the norm $\|f\|_{k,2} = \sum_{|\alpha| \le k} \|D^\alpha f\|_{L^2}$ is equivalent to the norm $\|f\|_k$ on W_k. By Leibnitz's rule and the fact that the derivatives of g are bounded we have

$$\|gf\|_{k,2} = \sum_{|\alpha| \le k} \|D^\alpha gf\|_2 \le C \sum_{|\alpha| \le k} \|D^\alpha f\|_2 = C\|f\|_{k,2}$$

Thus $g: W_k \to W_k$ is bounded. By duality, $g: W_{-k} \to W_{-k}$ is bounded. The spaces W_m are the rigged Hilbert spaces associated with the operator $-\Delta + I$, so by the interpolation theorem, $g: W_m \to W_m$ is bounded for each m with $|m| \le k$. ∎

For another application of the $\mathscr{H}_m$-interpolation theorem, see the proof of Theorem X.18. For another illustration of interpolating spaces, see Problem 36.

IX.5 Fundamental solutions of partial differential equations with constant coefficients

In this section and the next we will describe two applications of the Fourier transform to the study of partial differential equations. This is not a book about partial differential equations though we have touched on the subject from time to time, so our purpose here is neither to discuss in detail the techniques nor give the strongest results, but to illustrate and explain the application of the methods of functional analysis.

As in Chapter V, $p(x)$ denotes a polynomial in several variables $x = \langle x_1, \ldots, x_n\rangle$, and $p(D)$ denotes the partial differential operator obtained by substituting $\partial/\partial x_i$ for x_i wherever it occurs in $p(x)$.

Definition A **fundamental solution** for the partial differential operator $p(D)$ is a distribution $E \in \mathscr{D}'$ so that $p(D)E = \delta$.

The reason for studying fundamental solutions is that if we define $u = E * f$ where $f \in C_0^\infty(\mathbb{R}^n)$, then

$$\begin{aligned} p(D)u = p(D)(E * f) &= p(D)E * f \\ &= \delta * f \\ &= f \end{aligned}$$

Thus, if we can find a fundamental solution, then we have an existence theorem for all the partial differential equations $p(D)u = f$ where $f \in C_0^\infty(\mathbb{R}^n)$. Furthermore, if we can find an expression for E, then we have an explicit representation of a solution, namely $u = E * f$.

Example (Poisson's equation) For Poisson's equation, $\Delta u = f$, in three dimensions, the function $E(\mathbf{r}) = -1/4\pi r$ is a fundamental solution. This can be seen as follows: We denote by B_ε the ball about zero of radius ε. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$. Then

$$\begin{aligned} (\Delta E)(\varphi) = E(\Delta\varphi) &= -\int_{\mathbb{R}^3} \frac{1}{4\pi r} \Delta\varphi \, dx \\ &= \lim_{\varepsilon \downarrow 0} -\int_{\mathbb{R}^3 \setminus B_\varepsilon} \frac{1}{4\pi r} \Delta\varphi \, dx \\ &= \lim_{\varepsilon \downarrow 0} \left\{ \int_{\mathbb{R}^3 \setminus B_\varepsilon} -\Delta\left(\frac{1}{4\pi r}\right)\varphi \, dx + \int_{\partial B_\varepsilon} \frac{1}{4\pi r} \frac{\partial}{\partial r} \varphi \, dS - \int_{\partial B_\varepsilon} \varphi \frac{\partial}{\partial r}\left(\frac{1}{4\pi r}\right) dS \right\} \end{aligned}$$

where dS denotes the usual measure on the surface ∂B_ε of B_ε. The first term on the right-hand side equals zero. The second term converges to zero and the third term converges to $\varphi(0)$ as $\varepsilon \downarrow 0$ because φ is continuous at zero. Thus $\Delta E(\varphi) = \varphi(0)$ so $\Delta E = \delta$.

In order to see the difficulties in finding fundamental solutions, let us work formally for a moment. We would like to solve the partial differential equation $p(D)E = \delta$. Taking the Fourier transform of both sides we obtain $p(ix)\hat{E} = (2\pi)^{-n/2}$, so we expect

$$E = \widehat{((2\pi)^{n/2} p(ix))^{-1}}$$

If $p(ix)$ has no real zeros, then we can use the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$ to define E. However, $p(ix)$ is a polynomial in several variables and may have whole manifolds of zeros. Thus $p(ix)^{-1}$ may not be locally integrable in which case $\int p(ix)^{-1}\varphi(x)\,dx$ does not make sense as it stands,

so we cannot immediately interpret $p(ix)^{-1}$ as a distribution. This is reminiscent of the situation in Examples 6 and 9 of Section V.3 where the function $1/x$ in one variable could not be immediately interpreted as a distribution since it is not locally integrable. Even in that simple case, a limiting procedure was required. As in that case, we expect that different limiting procedures will give different distributions. In fact, in general, partial differential equations will have many fundamental solutions in $\mathscr{D}'$, and sometimes have more than one in $\mathscr{S}'(\mathbb{R}^n)$.

The Malgrange–Ehrenpreis theorem states that every constant coefficient partial differential operator $p(D)$ has a fundamental solution. The proof depends on a complex-variables argument and the Hahn–Banach theorem. Before giving a sketch of the proof, we will illustrate the Hahn–Banach part of the argument by a simple example. Consider the operator $I - \Delta$. In this case $p(ix) = 1 + x^2$ has no zeros, so $\hat{E} = \{(2\pi)^{n/2}(1 + x^2)\}^{-1}$ is a well-defined tempered distribution and E satisfies $(I - \Delta)E = \delta$. We now give another argument which proves the existence of E without using the fact that we have extended the Fourier transform to $\mathscr{S}'$. Let $\varphi \in C_0^\infty(\mathbb{R}^n)$. Then

$$\begin{aligned} |\delta_0(\varphi)| = |\varphi(0)| &\le \|\varphi\|_\infty \\ &\le \|\hat{\varphi}\|_1 \\ &= \|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)(1 + |\lambda|^2)^{-m}\|_1 \\ &\le C\|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)\|_2 \end{aligned}$$

where we have chosen m large enough so that $(1 + |\lambda|^2)^{-m} \in L^2(\mathbb{R}^n)$. Using (IX.1) and the Plancherel theorem, we have

$$\|(1 + |\lambda|^2)^m \hat{\varphi}(\lambda)\|_2 = \|(1 - \Delta)^m \varphi\|_2$$

and thus

$$|\varphi(0)| \le C\|(1 - \Delta)^m \varphi\|_2 \tag{IX.21}$$

Therefore, the map $\tilde{T}$ from $(I - \Delta)^m[C_0^\infty(\mathbb{R}^n)]$ to $\mathbb{C}$ given by

$$\tilde{T}: (1 - \Delta)^m \varphi \to \varphi(0)$$

is well defined and bounded in the L^2-norm. By the Hahn–Banach theorem $\tilde{T}$ can be extended from $(I - \Delta)^m C_0^\infty(\mathbb{R}^n)$ to a bounded linear functional T on all of $L^2(\mathbb{R}^n)$. It follows from the Riesz lemma that there is a $t(x) \in L^2(\mathbb{R}^n)$ so that

$$\begin{aligned} \delta(\varphi) = \varphi(0) = T((I - \Delta)^m \varphi) \\ = \int t(x)(1 - \Delta)^m \varphi \, dx \\ = [(1 - \Delta)^{m-1} T]((1 - \Delta)\varphi) \end{aligned}$$

If we set $E = (1 - \Delta)^{m-1}T$, then clearly $(1 - \Delta)E = \delta$.

We are ready to state the Malgrange–Ehrenpreis theorem and sketch the proof.

Theorem IX.23 For every constant coefficient partial differential operator, $p(D)$, on $\mathbb{R}^n$, there is a distribution $E \in \mathscr{D}'$ so that $p(D)E = \delta$.

Proof Define $p^*(x) = p(-x)$ and $q(x) = p^*(ix)$ and let $\varphi \in C_0^\infty(\mathbb{R}^n)$. From the Paley–Wiener theorem we know that for each $y \in \mathbb{R}^n$,

$$\widehat{(p^*(D)\varphi)}(y + \zeta) = \hat{\varphi}(y + \zeta)q(y + \zeta)$$

is an entire function of $\zeta \in \mathbb{C}^n$. Let $Q(x) = \sum_\alpha |D^\alpha q(x)|$; notice that Q is positive and bounded away from zero. The first step in the proof uses the Cauchy integral formula to show that

$$|Q(x)\hat{\varphi}(x)| \le C_1 \int_{|\zeta| \le \varepsilon} |\hat{\varphi}(x + \zeta)q(x + \zeta)|\, d^{2n}\zeta$$

$$= C_1 \int_{|\zeta| \le \varepsilon} |\widehat{p^*(D)\varphi}(x + \zeta)|\, d^{2n}\zeta$$

where C_1 depends on ε but is independent of φ and $d^{2n}\zeta$ is Lebesgue measure on $\mathbb{C}^n$. This complex-variable argument is outlined in Problem 41.

Using the above estimate, we have

$$|\varphi(0)| \le (2\pi)^{-n/2} \int_{\mathbb{R}^n} |\hat{\varphi}(y)|\, dy$$

$$\le C_2 \int_{\mathbb{R}^n} \left(\int_{|\zeta| \le \varepsilon} |\widehat{p^*(D)\varphi}(y + \zeta)|\, |Q(y)|^{-1}\, d^{2n}\zeta \right) dy$$

$$= C_2 \int_{\mathbb{R}^n} \int_{|\lambda|^2 + |\mu|^2 \le \varepsilon^2} |\widehat{p^*(D)\varphi}(y + \lambda + i\mu)|\, |Q(y)|^{-1}\, d\lambda\, d\mu\, dy$$

For $|\lambda| \le \varepsilon$, $Q(y + \lambda)(Q(y))^{-1} \le C_3$ independently of y, so

$$|\varphi(0)| \le C_4 \int_{\mathbb{R}^n} \int_{|\lambda|^2 + |\mu|^2 \le \varepsilon^2} |\widehat{p^*(D)\varphi}(y + \lambda + i\mu)|(Q(y + \lambda))^{-1}\, d\lambda\, d\mu\, dy$$

$$\le C_5 \int_{\mathbb{R}^n} \int_{|\mu|^2 \le \varepsilon^2} |\widehat{p^*(D)\varphi}(y + i\mu)|(Q(y))^{-1}\, d\mu\, dy \qquad \text{(IX.22)}$$

This estimate takes the place of the simple a priori estimate (IX.21) in the above example (all the C_i depend on ε but are independent of φ).

From here on the structure of the argument is the same as in the example. Let

$$\|\varphi\|_Q = \int_{\mathbb{R}^n} \int_{|\mu|^2 \le \varepsilon^2} |\hat{\varphi}(y + i\mu)(Q(y))^{-1}|\, d\mu\, dy$$

We first show that $\|\cdot\|_Q$ is a continuous norm on $\mathscr{D}$. Since Q is bounded from below

$$\|\varphi\|_Q \le C_6 \int_{\mathbb{R}^n} \int_{|\mu| \le \varepsilon} |\hat{\varphi}(y + i\mu)|\, d\mu\, dy$$

$$\le C_7 \sup_{\substack{y \in \mathbb{R}^n \\ |\mu| \le \varepsilon}} |(1 + y^2)^{n+1}\hat{\varphi}(y + i\mu)|$$

$$\le C_7 \sup_{|\mu| \le \varepsilon} \|(I - \Delta)^{n+1} e^{\mu \cdot x}\varphi(x)\|_1$$

The right-hand side is a continuous norm on $C_0^\infty(K)$ for each compact set $K \subset \mathbb{R}^n$. Since $\mathscr{D}$ has the inductive limit topology, $\|\cdot\|_Q$ is a continuous norm on $\mathscr{D}$. The basic estimate (IX.22) shows that the map

$$\tilde{E}\colon\ p^*(D)\varphi \to \varphi(0)$$

is well-defined. That is, if $p^*(D)\varphi_1 = p^*(D)\varphi_2$, then $\varphi_1(0) = \varphi_2(0)$. $\tilde{E}$ is continuous since $\|\cdot\|_Q$ is a continuous norm. Thus by the Hahn–Banach theorem there is an E in $\mathscr{D}'$ which extends $\tilde{E}$. Since

$$(p(D)E)(\varphi) = E(p^*(D)\varphi) = \varphi(0)$$

we have found a fundamental solution for $p(D)$. ∎

IX.6 Elliptic regularity

I turn away with fear and horror from this lamentable plague of functions which do not have derivatives. — *Hermite, in a letter to Stieltjes*

Suppose that u is a weak solution of $-\Delta u = g$ in a region Ω. Our main goal in this section is to prove that if g is C^∞ in Ω, then u is C^∞ in Ω also. This theorem, known as Weyl's lemma, has many important generalizations. We restrict ourselves here to a proof of Weyl's lemma, leaving a discussion of the generalizations to the notes. The importance of these so-called "regularity" theorems is that they provide the second step in the proof

that certain classes of elliptic partial differential equations have strict solutions. One first uses the Hahn–Banach theorem or a self-adjointness argument to prove the existence of a weak solution (see Section IX.5 or X.3), and then uses a regularity theorem to prove that any weak solution is a strict solution. In Section V.4 we noted that $u_{tt} - u_{xx} = 0$ has many weak solutions which are *not* strict solutions. The difference between the two cases $u_{tt} - u_{xx} = 0$ and $u_{tt} + u_{xx} = 0$ lies in the fact that the polynomials xt, x, t, and 1 can all be bounded by $C(x^2 + t^2)$ but not by $C(x^2 - t^2)$. The reader will see how such estimates enter into the proof. Although a regularity theorem of the C^∞-type (or even the C^k-type) does not hold for non-elliptic partial differential equations, there is a weaker regularity theorem which we discuss in the Notes to Section IX.10.

The proof of Weyl's lemma itself is divided into two parts. The first is to show that if $-\Delta u = g$ and if all the weak derivatives of g of order less than or equal to m are L^2 functions, then all the weak derivatives of u of order less than or equal to $m + 2$ are L^2 functions. The second part, known as Sobolev's lemma, shows that any function in $L^2(\mathbb{R}^n)$ which has $k > (n/2) + \sigma$ weak derivatives in $L^2(\mathbb{R}^n)$ is equal (a.e.) to a function in C^σ. Weyl's lemma results from combining these two parts with the assumption that g is C^∞.

We begin by introducing the Sobolev spaces and several of their important properties.

Definition A distribution $T \in \mathscr{S}'(\mathbb{R}^n)$ is said to be in W_m, the ***m*th Sobolev space** ($m \in \mathbb{R}$) if $\hat{T}$ is a measurable function and

$$\|T\|_m^2 = \int (1 + |\lambda|^2)^m |\hat{T}(\lambda)|^2 \, d\lambda < \infty$$

W_m is a Hilbert space under the norm $(T, T)^{1/2} = \|T\|_m$. As in the discussion of quadratic forms in Section VIII.6, it is useful to suppress the correspondence between W_m^* and W_m given by the Riesz lemma. Instead we identify W_m^* and W_{-m} by associating $T \in W_{-m}$ with the functional on W_m given by

$$T(S) = \int \hat{T}(-\lambda)\hat{S}(\lambda) \, d\lambda$$

This identification is natural since it agrees with the meaning of $T(\varphi)$ when $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and T is viewed as an element of $\mathscr{S}'(\mathbb{R}^n)$.

Proposition 1 If m is a nonnegative integer, then $f \in W_m$ if and only if $D^\alpha f \in L^2(\mathbb{R}^n)$ for all α satisfying $|\alpha| \leq m$, where $D^\alpha f$ means the derivative in the sense of distributions.

Proof By Theorem IX.2, $\widehat{D^\alpha T} = (i\lambda)^\alpha \hat{T}$ for all T in $\mathscr{S}'(\mathbb{R}^n)$. If $T \in W_m$, then $(i\lambda)^\alpha \hat{T} \in L^2(\mathbb{R}^n)$ if $|\alpha| \leq m$, so by the Plancherel theorem $D^\alpha T \in L^2(\mathbb{R}^n)$. Conversely, if $D^\alpha T \in L^2(\mathbb{R}^n)$ for all α with $|\alpha| \leq m$, then $(i\lambda)^\alpha \hat{T} = \widehat{D^\alpha T} \in L^2(\mathbb{R}^n)$ if $|\alpha| \leq m$, so $T \in W_m$. ∎

Proposition 2 Let m be an integer. If $T \in W_m$ and $\varphi \in C^{|m|}$ with bounded derivatives, then $\varphi T \in W_m$.

Proof If $m \geq 0$, then the conclusion follows from Leibnitz's rule and Proposition 1. If $m < 0$, multiplication by φ on W_m is the adjoint of multiplication by φ on $W_{|m|}$ under the natural identification of W_m and $W_{|m|}^*$. Thus multiplication by φ is bounded. ∎

The above proposition is a special case of Proposition 10 in the Appendix to Section IX.4. We have repeated the proof since this part of Proposition 10 does not need interpolation.

Definition Let Ω be an open subset of $\mathbb{R}^n$. The **local Sobolev space** $W_m(\Omega)$ is the set of distributions $T \in \mathscr{D}'(\mathbb{R}^n)$ so that $\varphi T \in W_m$ for all $\varphi \in C_0^\infty(\mathbb{R}^n)$ with support in Ω.

The useful property of the local Sobolev spaces is:

Proposition 3 If Ω is an open *bounded* region in $\mathbb{R}^n$, then every $T \in \mathscr{D}'(\mathbb{R}^n)$ is in $W_m(\Omega)$ for some m. That is, $\mathscr{D}'(\mathbb{R}^n) = \bigcup_{m=-\infty}^{\infty} W_m(\Omega)$.

Proof Let η be a function in $C_0^\infty(\mathbb{R}^n)$ which is identically one on $\overline{\Omega}$. Since ηT is a distribution with compact support, $|(\widehat{\eta T})(\lambda)| \leq C(1 + |\lambda|)^M$ for some M by Theorem IX.12. Thus, if p is an integer larger than $M + (n/2)$, $\eta T \in W_{-p}$. By Proposition 2, if $\varphi \in C_0^\infty(\mathbb{R}^n)$ with supp $\varphi \subset \Omega$, then $\varphi T = \varphi \eta T \in W_{-p}$ also. Thus $T \in W_{-p}(\Omega)$. ∎

We are now prepared for the first part of the proof of Weyl's lemma.

Lemma Let $T \in \mathscr{D}'(\mathbb{R}^n)$ and Ω be an open set in $\mathbb{R}^n$.

(a) If $T \in W_m$ and $-\Delta T \in W_m$, then $T \in W_{m+2}$. Furthermore, if $T \in W_m$, then $\partial T/\partial x_j \in W_{m-1}$.
(b) If $T \in W_m(\Omega)$ and $-\Delta T \in W_m(\Omega)$, then $T \in W_{m+2}(\Omega)$.
(c) If $T \in W_m$ and m is an integer, then $T \in W_m(\Omega)$.

Proof To prove (a), notice that if $T \in W_m$, then $(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n)$; and if $-\Delta T \in W_m$, then $|\lambda|^2(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n)$. Thus

$$(1 + |\lambda|^2)^{(m/2)+1}\hat{T} \in L^2(\mathbb{R}^n),$$

so $T \in W_{m+2}$. Further, if $T \in W_m$, then $\lambda_j(1 + |\lambda|^2)^{(m-1)/2}\hat{T} \in L^2(\mathbb{R}^n)$, so $\partial T/\partial x_j \in W_{m-1}$.

To prove (b), we first note that Leibnitz's rule holds for the product of a distribution and a function, i.e.

$$\frac{\partial}{\partial x_j}(\varphi T) = \left(\frac{\partial \varphi}{\partial x_j}\right)T + \varphi \frac{\partial T}{\partial x_j} \tag{IX.23}$$

$$-\Delta(\varphi T) = (-\Delta\varphi)T - 2\sum \frac{\partial \varphi}{\partial x_j}\frac{\partial T}{\partial x_j} - \varphi\, \Delta T \tag{IX.24}$$

Now, suppose T and $-\Delta T$ are in $W_m(\Omega)$. If $\varphi \in C_0^\infty(\Omega)$, then by (IX.23) and part (a), $\varphi\, \partial T/\partial x_j \in W_{m-1}$. Thus, by (IX.24), $-\Delta(\varphi T) \in W_{m-1}$, so by part (a) we conclude that $\varphi T \in W_{m+1}$. We now use (IX.23) again obtaining $\varphi\, \partial T/\partial x_j \in W_m$ and (IX.24) again obtaining $-\Delta(\varphi T) \in W_m$. Thus, it follows from part (a) that $\varphi T \in W_{m+2}$. Since $\varphi \in C_0^\infty(\Omega)$ was arbitrary, $T \in W_{m+2}(\Omega)$. This proves (b).

(c) follows from Proposition 2. ∎

Theorem IX.24 (Sobolev's lemma) Let $T \in \mathscr{D}'(\mathbb{R}^n)$ and let Ω be an open set in $\mathbb{R}^n$. Suppose that $T \in W_m(\Omega)$, where $m > n/2$ and let ℓ be a non-negative integer satisfying $\ell < m - (n/2)$. Then on Ω, T is equal to a C^ℓ function.

Proof We begin with the case where $\Omega = \mathbb{R}^n$. Since $T \in W_m$,

$$(1 + |\lambda|^2)^{m/2}\hat{T} \in L^2(\mathbb{R}^n).$$

Thus, since $(1 + |\lambda|^2)^{-(n/4)-\varepsilon}$ is also in $L^2(\mathbb{R}^n)$ for each $\varepsilon > 0$, we conclude that

$$(1 + |\lambda|^2)^{-(n/4)-\varepsilon}(1 + |\lambda|^2)^{m/2}\hat{T}(\lambda) \in L^1(\mathbb{R}^n)$$

Therefore, whenever $|\alpha| \le \ell$

$$|\lambda^\alpha \hat{T}(\lambda)| \le |\lambda|^\ell(1 + |\lambda|^2)^{-(m/2)+(n/4)+\varepsilon}G(\lambda)$$

where $G \in L^1(\mathbb{R}^n)$. Since we can choose $\varepsilon > 0$ so that $\ell < m - (n/2) - 2\varepsilon$, $\lambda^\alpha \hat{T} \in L^1(\mathbb{R}^n)$ for each $|\alpha| \le \ell$. By the Riemann–Lebesgue lemma,

$$T(x) = (2\pi)^{-n/2}\int e^{i\lambda \cdot x}\hat{T}(\lambda)\, d\lambda$$

and

$$\mathbf{S}(x) = (2\pi)^{-n/2}\int e^{i\lambda \cdot x}(i\lambda)\hat{T}(\lambda)\, d\lambda$$

are continuous $\mathbb{R}$- and $\mathbb{R}^n$-valued functions respectively. Moreover, by the dominated convergence theorem

$$\frac{T(x+h) - T(x) - h \cdot \mathbf{S}(x)}{|h|}$$

$$= (2\pi)^{-n/2}\int \left[\frac{e^{i\lambda \cdot (x+h)} - e^{i\lambda \cdot x} - i\lambda \cdot h\, e^{i\lambda \cdot x}}{|h|}\right]\hat{T}(\lambda)\, d\lambda$$

converges to zero as $|h| \downarrow 0$. Thus T is C^1 with $\mathbf{D}T = \mathbf{S}$. Using the fact that $(1 + |\lambda|^\ell)\hat{T} \in L^1(\mathbb{R}^n)$, we repeat this process ℓ times to conclude that $T(x)$ is ℓ times continuously differentiable.

We now treat the general case. Let η and ψ be in $C_0^\infty(\Omega)$ and suppose that both η and ψ equal one in a neighborhood N of a point $x \in \Omega$. Since $T \in W_m(\Omega)$, ψT and ηT are C^ℓ functions on $\mathbb{R}^n$. Furthermore we must have $(\psi T)(x) = (\eta T)(x)$ since otherwise we could find a φ with support in N so that $T(\varphi) = (\psi T)(\varphi) \neq (\eta T)(\varphi) = T(\varphi)$. Thus we can define a function $F(x) = (\psi T)(x)$ on Ω by letting ψ be any $C_0^\infty(\Omega)$ function that is one in a neighborhood of x. By what we proved above, $F(x)$ is ℓ times continuously differentiable.

We complete the proof by showing that in Ω, T is given by $F(x)$. Suppose $\varphi \in C_0^\infty(\Omega)$ and let $\alpha(x)$ be a function in $C_0^\infty(\Omega)$ which equals one on $\overline{\text{supp } \varphi}$. Then

$$T(\varphi) = T(\alpha\varphi) = (\alpha T)(\varphi) = \int_\Omega F(x)\varphi(x)\, dx \quad \blacksquare$$

Sobolev's lemma has extensions to various L^p spaces and under certain conditions to the case where $\ell = m - (n/2)$. These extensions are more difficult to prove and are discussed in the Notes.

Theorem IX.25 (Weyl's lemma) Let u be a weak solution of the equation $-\Delta u = g$ on $\mathbb{R}^n$. If g is a C^m function on an open set $\Omega \subset \mathbb{R}^n$, then on Ω, u is equal to a C^ℓ function for each $\ell \in I_+$ satisfying $\ell < m - (n/2) + 2$. In particular if g is C^∞ in Ω, then u is C^∞ in Ω.

Proof We may assume, without loss of generality, that Ω is bounded. Since $\varphi g \in W_m$ for each $\varphi \in C_0^\infty(\Omega)$, $g \in W_m(\Omega)$. By Theorem IX.23, $u \in W_k(\Omega)$ for some k since $u \in \mathscr{D}'(\mathbb{R}^n)$. If $k < m+2$, then, using the facts that $u \in W_k(\Omega)$, $-\Delta u = g \in W_k(\Omega)$, and the lemma, we conclude that $u \in W_{k+2}(\Omega)$. Repeating this process we obtain the result that $u \in W_{m+2}(\Omega)$ which implies by Sobolev's lemma that u is a C^ℓ function on Ω for $\ell < m - (n/2) + 2$. ∎

Theorem IX.26 (local regularity for Schrödinger's equation) Let u be a weak solution of the equation $(-\Delta + V)u = Eu$ where V is a measurable function and E is a complex number. Then, if V is equal to a C^∞ function in an open region Ω, u is C^∞ in that region also.

Proof Without loss we may suppose that Ω is bounded. Since $u \in \mathscr{D}'(\mathbb{R}^n)$, $u \in W_k(\Omega)$ for some k by Proposition 3. But, since V is C^∞, $Vu \in W_k(\Omega)$ by Proposition 2. Thus, $u \in W_k(\Omega)$ and $-\Delta u \in W_k(\Omega)$, so by the lemma, $u \in W_{k+2}(\Omega)$. By repeatedly using the lemma we find that $u \in \bigcap_{k=-\infty}^{\infty} W_k(\Omega)$ which implies by Sobolev's lemma that u is C^∞ in Ω. ∎

We remark that our method of proof of Theorem IX.26 can be extended to show that if $V \in C^m(\Omega)$, then $u \in C^\ell(\Omega)$ if $\ell < m - (n/2) + 2$ (Problem 45).

IX.7 The free Hamiltonian for nonrelativistic quantum mechanics

In this section we study $-\Delta$ as an operator on $L^2(\mathbb{R}^n)$. There are two reasonable domains to choose for $-\Delta$,

$$D_{\max} = \{\varphi \mid \varphi \in L^2(\mathbb{R}^n) \text{ and } \Delta\varphi \in L^2(\mathbb{R}^n) \text{ in the sense of distributions}\}$$

$$D_{\min} = C_0^\infty(\mathbb{R}^n)$$

We denote $-\Delta \upharpoonright D_{\max}$ by $T_{\max}$ and $-\Delta \upharpoonright D_{\min}$ by $T_{\min}$.

Theorem IX.27

(a) $\varphi \in D_{\max}$ if and only if $|\lambda|^2\hat{\varphi}(\lambda) \in L^2(\mathbb{R}^n)$ and in that case $T_{\max}\varphi = \widehat{|\lambda|^2\hat{\varphi}(\lambda)}$.

(b) $T_{\max}$ is self-adjoint.

(c) $T_{\min}$ is essentially self-adjoint and $\overline{T}_{\min} = T_{\max}$.

Proof (a) follows immediately from the formula $-\widehat{\Delta T} = |\lambda|^2\hat{T}$ which is valid for arbitrary tempered distributions. By Proposition 1 of Section VIII.3, multiplication by $|\lambda|^2$ is self-adjoint on $\{\varphi \in L^2(\mathbb{R}^n) \mid |\lambda|^2\varphi \in L^2(\mathbb{R}^n)\}$. Since $\mathscr{F}$ is unitary and $T_{\max} = \mathscr{F}^{-1}|\lambda|^2\mathscr{F}$, $T_{\max}$ is self-adjoint on $D_{\max}$.

To prove that $T_{\min}$ is essentially self-adjoint it is sufficient to show that $T_{\min}^* = T_{\max}$ since then $\overline{T}_{\min} = T_{\min}^{**} = T_{\max}$. Suppose that $\psi \in D(T_{\min}^*)$. Then $(-\Delta\varphi, \psi) = (T_{\min}\varphi, \psi) = (\varphi, T_{\min}^*\psi)$ for all $\varphi \in C_0^\infty(\mathbb{R}^n)$. Thus $-\Delta\psi \in L^2(\mathbb{R}^n)$ in the sense of distributions, so $\psi \in D_{\max}$ and $T_{\min}^*\psi = -\Delta\psi = T_{\max}\psi$. Conversely, suppose that $\psi \in D_{\max}$. Then $-\Delta\psi \in L^2(\mathbb{R}^n)$ so that for all $\varphi \in C_0^\infty$, $(-\Delta\varphi, \psi) = (\varphi, -\Delta\psi)$. Thus, $\psi \in D(T_{\min}^*)$ and $T_{\min}^*\psi = -\Delta\psi$. ∎

Definition We denote $-\Delta$ with the domain $D_{\max}$ by H_0 and call it the **free Hamiltonian**.

In the remainder of this section we use the Fourier transform and the estimates in Section IX.4 to study various properties of H_0. First we prove a theorem that gives further properties of the functions in $D(H_0)$. Then we derive explicit formulas for $R_\lambda(H_0)$ and e^{itH_0}. Finally, we prove some asymptotic properties of e^{itH_0} which will be useful when we treat scattering theory in Chapter XII.

Since H_0 is self-adjoint, its powers H_0^m are also self-adjoint. Since $H_0^m = \mathscr{F}^{-1}|\lambda|^{2m}\mathscr{F}$, the domain of H_0^m is just the Sobolev space W_{2m} introduced in Section IX.6. Sobolev's lemma (Theorem IX.24) immediately implies:

Proposition A vector $\varphi \in L^2(\mathbb{R}^n)$ is in $C^\infty(H_0) = \bigcap_{m=1}^{\infty} D(H_0^m)$ if and only if $\varphi \in C^\infty(\mathbb{R}^n)$ and $D^\alpha\varphi \in L^2(\mathbb{R}^n)$ for each α.

More importantly, the vectors in $D(H_0)$ itself have the following properties:

Theorem IX.28 Let $\varphi \in L^2(\mathbb{R}^n)$ be in $D(H_0)$. Then

(a) If $n \leq 3$, φ is a bounded continuous function and for any $a > 0$, there is a b, independent of φ, so that

$$\|\varphi\|_\infty \leq a\|H_0\varphi\| + b\|\varphi\| \tag{IX.25}$$

(b) If $n \geq 4$ and $2 \leq q < 2n/(n-4)$, then $\varphi \in L^q(\mathbb{R}^n)$ and for any $a > 0$ there is a b (depending only on q, n, and a) so that

$$\|\varphi\|_q \leq a\|H_0\varphi\| + b\|\varphi\| \tag{IX.26}$$

Proof By the Riemann–Lebesgue lemma and the Plancherel theorem, (a) will follow if we can prove that $\hat{\varphi} \in L^1(\mathbb{R}^n)$ and

$$\|\hat{\varphi}\|_1 \leq a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2 \tag{IX.27}$$

We will prove (IX.27) in the case $n = 3$. Suppose $\varphi \in D(H_0)$, then $(1 + \lambda^2)\hat{\varphi}$ and $(1 + \lambda^2)^{-1}$ are in $L^2(\mathbb{R}^3)$ so $\hat{\varphi} \in L^1(\mathbb{R}^3)$ and by the Schwarz inequality

$$\|\hat{\varphi}\|_1 \leq c\|(\lambda^2 + 1)\hat{\varphi}\|_2 \leq c(\|\lambda^2\hat{\varphi}\|_2 + \|\hat{\varphi}\|_2) \tag{IX.28}$$

where $c^2 = \int (1 + \lambda^2)^{-2}\, d\lambda$. For any $r > 0$, let $\hat{\varphi}_r(\lambda) = r^3\hat{\varphi}(r\lambda)$. Then $\|\hat{\varphi}_r\|_1 = \|\hat{\varphi}\|_1$, $\|\hat{\varphi}_r\|_2 = r^{3/2}\|\hat{\varphi}\|_2$, and $\|\lambda^2\hat{\varphi}_r\|_2 = r^{-1/2}\|\lambda^2\hat{\varphi}\|_2$. Thus, using (IX.28) for $\hat{\varphi}_r$, and using these equalities, we obtain

$$\|\hat{\varphi}\|_1 \leq cr^{-1/2}\|\lambda^2\hat{\varphi}\|_2 + cr^{3/2}\|\hat{\varphi}\|_2$$

for any $r > 0$. If we choose r large enough, (IX.27) follows.

By the Hausdorff–Young inequality and the Plancherel theorem, in order to prove (b) we need only show that for any p satisfying $2n/(n + 4) < p \leq 2$ and $a > 0$ there is a b so that

$$\|\hat{\varphi}\|_p \leq a\|\lambda^2\hat{\varphi}\|_2 + b\|\hat{\varphi}\|_2$$

The Hölder inequality implies that

$$\|\hat{\varphi}\|_p^p \leq \|(1 + \lambda^2)^{-p}\|_r \|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s$$

where $r^{-1} + s^{-1} = 1$. Choosing $s = 2/p$, the triangle inequality shows that

$$\begin{aligned}\|(1 + \lambda^2)^p|\hat{\varphi}|^p\|_s &= (\|(1 + \lambda^2)|\hat{\varphi}|\,\|_2)^p \\ &\leq (\|\hat{\varphi}\|_2 + \|\lambda^2\hat{\varphi}\|_2)^p\end{aligned}$$

Thus if $\|(1 + \lambda^2)^{-p}\|_{2(2-p)^{-1}} = c_1 < \infty$, we have

$$\|\hat{\varphi}\|_p \leq c_1^{1/p}(\|\lambda^2\hat{\varphi}\|_2 + \|\hat{\varphi}\|_2)$$

But

$$\|(1 + \lambda^2)^{-p}\|_{2(2-p)^{-1}}^{2(2-p)^{-1}} = \int \frac{d\lambda}{(1 + \lambda^2)^{2p(2-p)^{-1}}} < \infty$$

if $4p(2 - p)^{-1} > n$, i.e. if $p > 2n/(4 + n)$. The method of proving that the constant in front of $\|\lambda^2\hat{\varphi}\|$ can be chosen arbitrarily small is the same as in part (a). ∎

We will see in Section X.2 that part (b) of the theorem holds in the case $n \geq 5$ and $q = 2n/(n - 4)$ for some fixed a.

We turn now to computing explicit formulas for $(H_0 - E)^{-1}$, $E \in \mathbb{C}\backslash[0, \infty)$, and e^{-iH_0t}, $\operatorname{Im} t \leq 0$. Since $H_0 = \mathscr{F}^{-1}\lambda^2\mathscr{F}$, $f(H_0) = \mathscr{F}^{-1}f(\lambda^2)\mathscr{F}$ where f is any bounded measurable function. That is, both $(H_0 - E)^{-1}$ and e^{-iH_0t} can be expressed in terms of multiplication operators:

$$(H_0 - E)^{-1} = \mathscr{F}^{-1}(\lambda^2 - E)^{-1}\mathscr{F}; \qquad e^{-iH_0t} = \mathscr{F}^{-1}e^{-i\lambda^2t}\mathscr{F}$$

Since the Fourier transform takes multiplication into convolution, we will get simple expressions for $(H_0 - E)^{-1}$ and e^{-iH_0t} as convolution operators.

Let $f \in L^\infty(\mathbb{R}^n)$; we denote the operator $\varphi \mapsto (\widetilde{f\hat{\varphi}})$ on $L^2(\mathbb{R}^n)$ by $f(-i\nabla)$. Notice that $f(-i\nabla)$ is a well-defined bounded operator since multiplication by f is bounded.

Theorem IX.29 Let $f \in L^\infty(\mathbb{R}^n)$. If either (i) $f \in L^2(\mathbb{R}^n)$ *or* (ii) $\check{f} \in L^1(\mathbb{R}^n)$, then

$$(f(-i\nabla)\varphi)(x) = (2\pi)^{-n/2}\int \check{f}(x - y)\varphi(y)\, dy \tag{IX.29}$$

for all $\varphi \in L^2(\mathbb{R}^n)$. The integral converges for all x in case (i) and for almost all x in case (ii).

Proof Suppose $f \in L^2 \cap L^\infty$ and $\varphi \in \mathscr{S}$. Then $f \in \mathscr{S}'$ so by Theorem IX.4,

$$\begin{aligned}f(-i\nabla)\varphi \equiv (\widetilde{f\hat{\varphi}}) &= (2\pi)^{-n/2}\check{f} * \varphi \\ &= (2\pi)^{-n/2}\int \check{f}(y)\varphi(x - y)\, dy\end{aligned}$$

so (IX.29) holds if $\varphi \in \mathscr{S}$. For $\varphi \in L^2(\mathbb{R}^n)$, we can find a sequence $\varphi_m \in \mathscr{S}$ so that $\varphi_m \xrightarrow{L^2} \varphi$. Since $f \in L^\infty$, $f\hat{\varphi}_m \xrightarrow{L^2} f\hat{\varphi}$, so $f(-i\nabla)\varphi_m \to f(-i\nabla)\varphi$. Thus we can find a subsequence (which we also call $\{\varphi_m\}$) so that $f(-i\nabla)\varphi_m \to f(-i\nabla)\varphi$ pointwise a.e. Since $\check{f} \in L^2(\mathbb{R}^n)$,

$$\begin{aligned}\lim_{m\to\infty}(f(-i\nabla)\varphi_m)(x) &= \lim_{m\to\infty}(2\pi)^{-n/2}\int \check{f}(x - y)\varphi_m(y)\, dy \\ &= (2\pi)^{-n/2}\int \check{f}(x - y)\varphi(y)\, dy\end{aligned}$$

for each $x \in \mathbb{R}^n$. We have thus proven IX.29 in case (i).

To prove (IX.29) in case (ii), observe that if f_m and φ are in $\mathscr{S}(\mathbb{R}^n)$, then

$f_m(-i\nabla)\varphi = (2\pi)^{-n/2}\check{f}_m * \varphi$. Choose $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\check{f}_m \xrightarrow{L^1} \check{f}$. Then $f_m \xrightarrow{L^\infty} f$, so $f_m\hat{\varphi} \xrightarrow{L^2} f\hat{\varphi}$. Thus

$$\begin{aligned} f(-i\nabla)\varphi &= \lim_{m\to\infty} (2\pi)^{-n/2}\check{f}_m * \varphi \\ &= (2\pi)^{-n/2}\check{f} * \varphi \end{aligned}$$

by Young's inequality. Since the bounded operators, $f(-i\nabla)$ and convolution by $(2\pi)^{-n/2}\check{f}$ agree on $\mathscr{S}$, they agree on all of $L^2(\mathbb{R}^n)$. That the convolution, $\check{f} * \varphi$, is given by an absolutely convergent integral is proven in Example 1 of Section IX.4. ∎

Example 1 (the free resolvent, $n = 3$) Let $E = -\kappa^2$, where $\operatorname{Re}\kappa > 0$. Thus $E \in \rho(H_0)$. Since $f(\lambda) \equiv (\lambda^2 + \kappa^2)^{-1} \in L^2(\mathbb{R}^3) \cap L^\infty(\mathbb{R}^3)$, we can use part (i) of Theorem IX.29 to compute $(H_0 - E)^{-1}$. Since $f \in L^2$,

$$(2\pi)^{-3/2}\check{f}(x) = \operatorname*{l.i.m.}_{R\to\infty} (2\pi)^{-3}\int_{|\lambda|\le R} \frac{e^{i\lambda\cdot x}}{\lambda^2 + \kappa^2}\, d\lambda$$

Changing to spherical coordinates, set $u = \cos\sigma = \lambda\cdot x/|x||\lambda|$ and $r = |\lambda|$. Then

$$\begin{aligned} (2\pi)^{-3/2}\check{f}(x) &= \operatorname*{l.i.m.}_{R\to\infty} (2\pi)^{-2}\int_0^R\int_{-1}^1 \frac{e^{ir|x|u}}{r^2+\kappa^2}\, r^2\, dr\, du \\ &= \operatorname*{l.i.m.}_{R\to\infty} \frac{(2\pi)^{-2}}{i|x|}\int_{-R}^R \frac{e^{ir|x|}r}{r^2+\kappa^2}\, dr \\ &= \operatorname*{l.i.m.}_{R\to\infty} \frac{(2\pi)^{-2}}{i|x|}\int_{C_R} \frac{\tilde{r}e^{i\tilde{r}|x|}}{(\tilde{r}+i\kappa)(\tilde{r}-i\kappa)}\, d\tilde{r} \end{aligned}$$

where $\tilde{r}$ is in the complex r plane and C_R is the curve shown in

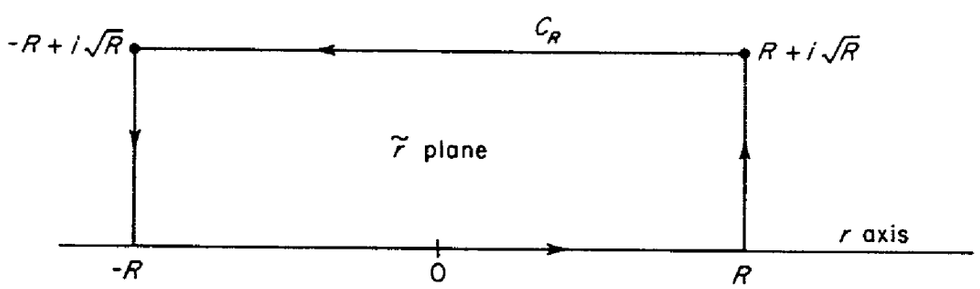


FIGURE IX.5 The path C_R.

Figure IX.5. For each $|x|$ the limit exists and equals $e^{-\kappa|x|}/4\pi|x|$. Thus, from Theorem IX.29 we have

$$(n = 3) \qquad [(H_0 + \kappa^2)^{-1}\varphi](x) = (4\pi)^{-1}\int \frac{e^{-\kappa|x-y|}}{|x-y|}\varphi(y)\, dy \qquad \text{(IX.30)}$$

The function $G_0(x, y; E) = e^{-\kappa|x-y|}/4\pi|x-y|$ is often called the **free Green's function.**

Example 2 (the free resolvent, $n \neq 3$) If n does not equal one or three, the computation of the inverse Fourier Transform of $(\lambda^2 + \kappa^2)^{-1}$ is not as explicit as in Example 1; it turns out to be an expression in terms of Bessel functions. It is not hard to see, however, that if $f(\lambda) = (\lambda^2 + \kappa^2)^{-1}$, then $\check{f} \in L^1(\mathbb{R}^n)$ (see Example 6 in Section IX.10 and Problem 49). Thus, we are in case (ii) of Theorem IX.29. Additional properties of Green's functions are given in Problem 49.

Example 3 (the free propagator) We want to compute an explicit formula for e^{-iH_0t}, $t \in \mathbb{R}$, the unitary group which gives the free quantum dynamics. $e^{-i\lambda^2 t}$ does not satisfy either of the criteria in Theorem IX.29 so we proceed as follows: Suppose that $\alpha \in \mathbb{C}$ and $\operatorname{Re}\alpha > 0$. Then

$$e^{-\lambda^2\alpha} \in L^2(\mathbb{R}^n) \cap L^\infty(\mathbb{R}^n)$$

so

$$(e^{-H_0\alpha}\varphi)(x) = \left(\frac{1}{4\pi\alpha}\right)^{n/2}\int e^{-|x-y|^2/4\alpha}\varphi(y)\, dy$$

since $\mathscr{F}^{-1}(e^{-\lambda^2\alpha}) = (2\alpha)^{-n/2}e^{-x^2/4\alpha}$ (Example 1 of Section IX.1). Now, suppose that $\varphi \in L^1 \cap L^2$. Since $e^{-i(t-i\varepsilon)H_0}\varphi \xrightarrow{L^2} e^{-itH_0}\varphi$ as $\varepsilon \downarrow 0$, we can find a subsequence which converges pointwise a.e. Thus

$$\begin{aligned} (e^{-itH_0}\varphi)(x) &= \lim_{\varepsilon\downarrow 0}(e^{-i(t-i\varepsilon)H_0}\varphi)(x) \\ &= \lim_{\varepsilon\downarrow 0}(4\pi i(t-i\varepsilon))^{-n/2}\int e^{-|x-y|^2/4i(t-i\varepsilon)}\varphi(y)\, dy \\ &= (4\pi it)^{-n/2}\int e^{i|x-y|^2/4t}\varphi(y)\, dy \end{aligned}$$

by the dominated convergence theorem. For general $\varphi \in L^2(\mathbb{R}^n)$, we can now use the trick employed in Section IX.2 to conclude that

$$(e^{-itH_0}\varphi)(x) = \operatorname{l.i.m.}(4\pi it)^{-n/2}\int e^{i|x-y|^2/4t}\varphi(y)\, dy \qquad \text{(IX.31)}$$

The function $P_0(x, y; t) = (4\pi it)^{-n/2} e^{i|x-y|/4t}$ is often called the **free propagator**.

To show how useful these explicit formulas are, we will derive two consequences of (IX.31) which are useful in scattering theory. The first is an estimate reflecting the spreading of free wave packets.

Theorem IX.30 Let H_0 be the free Hamiltonian on $\mathbb{R}^n$. Let $2 \le q \le \infty$ and $p = (1 - q^{-1})^{-1}$. Then

$$\|e^{-itH_0}\varphi\|_q \le t^{-n(p^{-1}-1/2)} \|\varphi\|_p \tag{IX.32}$$

Proof Since e^{-itH_0} is unitary on $L^2(\mathbb{R}^n)$, $\|e^{-itH_0}\varphi\|_2 = \|\varphi\|_2$. If $\varphi \in L^1 \cap L^2$, then it follows from (IX.31) that $\|e^{-itH_0}\varphi\|_\infty \le (4\pi t)^{-n/2} \|\varphi\|_1$. By the Riesz–Thorin theorem, e^{-itH_0} extends uniquely to a map from $L^p(\mathbb{R}^n)$ to $L^q(\mathbb{R}^n)$ and the estimate (IX.32) holds. ∎

The second application of (IX.31) is to prove an explicit asymptotic formula for e^{-itH_0}.

Theorem IX.31 Let H_0 be the free Hamiltonian on $\mathbb{R}^n$ and suppose $\varphi \in L^2(\mathbb{R}^n)$. Then

$$(e^{-itH_0}\varphi)(x) \to (2it)^{-n/2} e^{ix^2/4t} \hat{\varphi}(x/2t) \tag{IX.33}$$

in the sense that the difference goes to zero in L^2-norm as $t \to \infty$.

Proof For fixed t, the map V_t: $\varphi \to (2it)^{-n/2} e^{ix^2/4t} \hat{\varphi}(x/2t)$ is unitary so we need only prove the statement of the theorem for $\varphi \in \mathcal{S}$ and then use an $\varepsilon/3$ argument. Since

$$e^{i|x-y|^2/4t} = e^{ix^2/4t} e^{-ix \cdot y/2t} e^{iy^2/4t}$$

from (IX.31) we have

$$(e^{-iH_0t}\varphi)(x) - (V_t\varphi)(x) = (4\pi it)^{-n/2} e^{ix^2/4t} \int (e^{iy^2/4t} - 1) e^{-ix \cdot y/2t} \varphi(y)\, dy$$

$$= \frac{e^{ix^2/4t}}{(2it)^{n/2}} \hat{G}_t\left(\frac{x}{2t}\right)$$

where $G_t(y) = (e^{iy^2/4t} - 1)\varphi(y)$. Thus

$$\begin{aligned} \|e^{-iH_0t}\varphi - V_t\varphi\|_2 &= (2t)^{-n/2} \|\hat{G}_t(\cdot/2t)\|_2 \\ &= \|\hat{G}_t(\cdot)\|_2 \\ &= \|G_t\|_2 \\ &\le \frac{1}{4t} \|y^2\varphi(y)\|_2 \\ &\to 0 \qquad \text{as} \quad t \to \infty \end{aligned}$$

In the last step we used the estimate

$$|e^{iy^2/4t} - 1| = \left| \int_0^{y^2/4t} \frac{d}{dx}(e^{ix})\, dx \right| \le \frac{y^2}{4t} \quad ∎$$

Formula (IX.33) has a simple physical interpretation. To see this, we reintroduce the mass m by taking $H_0 = (-1/2m)\Delta$. If the system is in state φ at $t = 0$, then by (IX.33) the asymptotic probability density for position is $(m/t)^n |\hat{\varphi}(mx/t)|^2$. But $|\hat{\varphi}(\lambda)|^2$ is the initial probability density for momentum. Thus, for large times, the probability of a particle being at x at time t is proportional to the probability of its having momentum mx/t initially. So, for large times, the quantum free particle behaves like a classical free particle starting at $x = 0$ at time $t = 0$ with momentum density $|\hat{\varphi}(\lambda)|^2$.

IX.8 The Gårding–Wightman axioms

In this section we discuss several applications of the Fourier transform to the theory of quantized fields. It is not necessary for the reader to have had any previous experience with quantum field theory. We begin with a brief history, state the Wightman axioms, and define the Wightman functions. Then we use the Fourier transform to prove analyticity properties of the Wightman functions, outline the proof of the PCT theorem, and derive the Källen–Lehmann representation for the two-point function. In an appendix, we discuss Lorentz invariant measures.

Quantum field theory began in the twenties as an attempt to combine quantum mechanics and special relativity in a quantum generalization of the classical models for electromagnetic phenomena. Since then, field theory

has been used extensively to construct models for many elementary particle phenomena. From the beginning, it was apparent to the founders of the subject (Heisenberg, Pauli, Dirac) that there were many mathematical difficulties in the theory. Nevertheless, field theory continued to grow and by the forties had become a maze of folk theorems, conjectures, and complicated perturbation theory calculations, all difficult to prove since the central objects of the theory, the fields themselves, were only vaguely defined. Despite the fact that the theory lacked sound mathematical foundations, Schwinger, Feynman, Tomonaga, Dyson, and others systematized perturbation theory in the late 1940's to make calculations about electrodynamics. The striking experimental verification of these calculations suggested that within quantum field theory there were sound mathematical models for at least some elementary particle phenomena.

It was in this atmosphere that Gårding and Wightman formulated a definition of "quantum field" by proposing a set of mathematical properties which they argued every quantum field theory should possess. These properties are called **Wightman axioms**. The study of the Wightman axioms and their mathematical consequences is usually called **axiomatic quantum field theory**. This name is somewhat misleading for it has given many people the mistaken impression that the main interest is the axioms themselves rather than their mathematical consequences and the construction of specific examples. For this reason the subject is sometimes called "the general theory of quantized fields."

For simplicity we will only give the axioms for a "Hermitian scalar quantum field theory"; other cases are mentioned in the notes. We use units where the rationalized Planck's constant and the velocity of light are equal to one. Since we discuss each property briefly the definition is rather spread out.

*A **Hermitian scalar quantum field theory** is a quadruple $\langle \mathscr{H}, U, \varphi, D \rangle$ which satisfies the following properties* (1–8):

Property 1 (***relativistic invariance of states***) *$\mathscr{H}$ is a separable Hilbert space and $U(\cdot, \cdot)$ is a strongly continuous unitary representation on $\mathscr{H}$ of the restricted Poincaré group.*

The restricted Poincaré group is defined as follows: Let $x = \langle x^0, x^1, x^2, x^3 \rangle$ and $y = \langle y^0, y^1, y^2, y^3 \rangle$ be two vectors in $\mathbb{R}^4$. The Lorentz scalar product of x and y is defined to be $x^0y^0 - x^1y^1 - x^2y^2 - x^3y^3$. x^0 is called the time component of x; $\langle x^1, x^2, x^3 \rangle$ is called the space component. We denote by x_μ the components of the vector $\tilde{x} = (x^0, -x^1, -x^2, -x^3)$ so the Lorentz scalar product of x and y is just the usual inner product of x and $\tilde{y}$. Using the Einstein convention we will sometimes write the sum $\sum_{\mu=0}^{3} x^\mu y_\mu$ simply as $x^\mu y_\mu$, the summation being understood. The **Lorentz group** $\mathscr{L}$ is the set of linear transformations on $\mathbb{R}^4$ that preserve the Lorentz scalar product. The **restricted Lorentz group** $\mathscr{L}_+^\uparrow$ is the subgroup of those $\Lambda \in \mathscr{L}$ with $\det \Lambda = 1$ and with the matrix element between $\langle 1, 0, 0, 0 \rangle$ and itself positive. The **restricted Poincaré group** $\mathscr{P}_+^\uparrow$, is the set of pairs $\langle a, \Lambda \rangle$ where $a \in \mathbb{R}^4$ and $\Lambda \in \mathscr{L}_+^\uparrow$ with the group operation

$$\langle a, \Lambda_1 \rangle \langle b, \Lambda_2 \rangle = \langle a + \Lambda_1 b, \Lambda_1 \Lambda_2 \rangle$$

$\mathscr{P}_+^\uparrow$ acts naturally on $\mathbb{R}^4$ by $\langle a, \Lambda \rangle x = \Lambda x + a$ and is sometimes called the family of relativistic transformations of $\mathbb{R}^4$.

If we fix $\Lambda = I$, then $U(a) = U(a, I)$ is a strongly continuous unitary representation of $\mathbb{R}^4$. From Theorem VIII.12 if follows that there are four commuting self-adjoint operators P_0, P_1, P_2, P_3 on $\mathscr{H}$ and a projection-valued measure E_Ω on $\mathbb{R}^4$ so that

$$(\varphi, U(a)\varphi) = (\varphi, \exp(ia^\mu P_\mu)\varphi) = \int_{\mathbb{R}^4} e^{ia^\mu \lambda_\mu} \, d(\varphi, E_\lambda \varphi) \qquad \text{(IX.34)}$$

P_0 is called the **Hamiltonian** (or energy operator); P_j, $j = 1, 2, 3$, are the **momentum** operators.

Property 2 (***spectral condition***) *The projection-valued measure E_Ω on $\mathbb{R}^4$ corresponding to $U(a, I) = e^{ia^\mu P_\mu}$ has support in the closed forward light cone.*

The closed forward light cone is the set $V_+ = \{x \mid x \cdot \tilde{x} \geq 0, x^0 \geq 0\}$. Its interior will be denoted by V_+. The spectral condition is equivalent to the condition that the operators P_0 and $P_0^2 - P_1^2 - P_2^2 - P_3^2$ are both positive.

Property 3 (***existence and uniqueness of the vacuum***) *There exists a unique vector $\psi_0 \in \mathscr{H}$ so that $U(a, I)\psi_0 = \psi_0$ for all $a \in \mathbb{R}^4$. ψ_0 is called the **vacuum**.*

Property 3 implies that the point $\langle 0, 0, 0, 0 \rangle$ has nonzero E_Ω-measure and that $E_{\langle 0,0,0,0 \rangle}$ has a one-dimensional range. The $U(0, \Lambda)$ leave Ran $E_{\langle 0,0,0,0 \rangle}$ invariant so $U(0, \Lambda) \restriction \text{Ran } E_{\langle 0,0,0,0 \rangle}$ is a one-dimensional representation of $\mathscr{L}_+^\uparrow$. Since the only one-dimensional representation of $\mathscr{L}_+^\uparrow$ is the identity representation, it follows that $U(a, \Lambda)\psi_0 = \psi_0$ for all $\langle a, \Lambda \rangle \in \mathscr{P}_+^\uparrow$.

Property 4 (***invariant domains for fields***) *There is a dense subspace $D \subset \mathscr{H}$ and a map φ from $\mathscr{S}(\mathbb{R}^4)$ to the (unbounded) operators on $\mathscr{H}$ so that*

(i) For each $f \in \mathscr{S}(\mathbb{R}^4)$, $D \subset D(\varphi(f))$, $D \subset D(\varphi(f)^*)$ and $\varphi(f)^* \restriction D = \varphi(\bar{f}) \restriction D$.
(ii) $\psi_0 \in D$ and $\varphi(f)D \subset D$ for all $f \in \mathscr{S}(\mathbb{R}^4)$.
(iii) For fixed $\psi \in D$, the map $f \mapsto \varphi(f)\psi$ is linear.

Early formulations of field theory treated φ as an operator-valued function though the founders of the subject were aware that $\varphi(x)$ was a very singula object. The operator $\varphi(x)$ was said to be the "field at the point x" analogously to the classical electromagnetic field. This formulation led tc various difficulties which were overcome by taking the field φ to be ar operator-valued distribution rather than an operator-valued function; i.e., φ is defined on $\mathscr{S}(\mathbb{R}^4)$ rather than on $\mathbb{R}^4$. $\varphi(f)$ should be thought of as the space–time average of the hypothetical $\varphi(x)$ with the averaging function f. Symbolically

$$\varphi(f) = \int_{\mathbb{R}^4} \varphi(x) f(x)\, dx.$$

Bohr and Rosenfeld pointed out that from a physical point of view it is impossible to measure the electric field strength at a point because of certain quantum-mechanical effects related to the uncertainty principle. So, from a mathematical and a *physical* point of view it is reasonable to consider the **smeared field** $\varphi(f)$. In fact, it can be shown (Problem 53) that in a quantum field theory satisfying Properties 1–8, the field $\varphi(f)$ cannot arise from integrating a well-defined operator-valued function $\varphi(x)$ against $f(x)$.

The choice of $\mathscr{S}(\mathbb{R}^4)$ as a test function space for $\varphi(\cdot)$, rather than $C_0^\infty(\mathbb{R}^4)$ or some other test function space, is not absolutely necessary. Jaffe has made a detailed study of this question (see the Notes). The reason that we require (ii) is so that the **vacuum expectation values** $(\psi_0, \varphi(f_1) \cdots \varphi(f_n)\psi_0)$ make sense. One might suppose that it would be more useful to assume that $\varphi(f)$ is essentially self-adjoint on D rather than just symmetric, but this extra assumption seems to have few consequences.

Property 5 (***regularity of the field***) *For any ψ_1 and ψ_2 in D, the map $f \mapsto (\psi_1, \varphi(f)\psi_2)$ is a tempered distribution.*

The stronger statement that for $\psi \in D$, $f \mapsto \varphi(f)\psi$ is strongly continuous is a consequence of Properties 4 and 5 (Problem 54).

Property 6 (***Poincaré invariance of the field***) *For each $\langle a, \Lambda \rangle \in \mathscr{P}_+^\uparrow$, $U(a, \Lambda)D \subset D$ and for all $f \in \mathscr{S}(\mathbb{R}^4)$, $\psi \in D$,*

$$U(a, \Lambda)\varphi(f)U(a, \Lambda)^{-1}\psi = \varphi(\langle a, \Lambda \rangle f)\psi$$

where

$$\langle a, \Lambda \rangle f(x) = f(\Lambda^{-1}(x - a))$$

The invariance condition is often written formally as

$$U(a, \Lambda)\varphi(x)U(a, \Lambda)^{-1} = \varphi(\Lambda x + a)$$

Property 7 (***local commutativity or microscopic causality***) *If f and g in $\mathscr{S}(\mathbb{R}^4)$ have supports which are spacelike separated, then*

$$[\varphi(f)\varphi(g) - \varphi(g)\varphi(f)]\psi = 0$$

for all $\psi \in D$.

Two sets $S_1, S_2 \subset \mathbb{R}^4$ are called **spacelike separated** if $x \in S_1$ and $y \in S_2$ implies that $(x - y) \cdot (\widetilde{x - y}) < 0$. Property 7 expresses mathematically the quantum-mechanical statement that measurements in spacelike separated regions should not interfere with each other.

Property 8 (***cyclicity of the vacuum***) *The set D_0 of finite linear combinations of vectors of the form $\varphi(f_1) \cdots \varphi(f_n)\psi_0$ is dense in $\mathscr{H}$.*

This property ensures that the Hilbert space $\mathscr{H}$ is not too large, or put another way that the theory can be described in terms of a single field φ.

This completes the definition of a Hermitian scalar quantum field theory. There are two ways in which a mathematical investigation can now proceed. First, one can investigate the consequences of these axioms. The main bulk of the work in axiomatic field theory in the fifties and early sixties was of this type. In the remainder of this section we will show how the Fourier transform is used in deriving consequences of the axioms. The second general problem is to construct models satisfying all (or at least some) of the axioms. It was known when the axioms were formulated that they were consistent since the theory of free fields (see Section X.7) satisfies all the properties. Unfortunately, free field theories describe systems of particles that do not interact. It has proven very difficult to construct interesting

(i.e. interacting) examples. Some progress has been made on this problem in recent years (see Section X.7 and Chapter XIX).

We begin our discussion of the consequences of the axioms by defining the functionals

$$\mathscr{W}_n(f_1, \ldots, f_n) = (\psi_0, \varphi(f_1) \cdots \varphi(f_n)\psi_0)$$

The $\{\mathscr{W}_n\}$ are called **Wightman functions** or **Wightman distributions** or **vacuum expectation values**; $\mathscr{W}_n$ is sometimes called the ***n*-point function**. We will see in Chapter XVII that a field theory can be recovered from a knowledge of its Wightman functions. Let $\psi_1 = \varphi(\bar{f}_{k-1}) \cdots \varphi(\bar{f}_1)\psi_0$ and $\psi_2 = \varphi(f_{k+1}) \cdots \varphi(f_n)\psi_0$. Then by Property 4, ψ_1 and ψ_2 are in D so by Property 5 $\mathscr{W}_n(f_1, \ldots, f_n) = (\psi_1, \varphi(f_k)\psi_2)$ is continuous in f_k when the other f's are held fixed. Thus, $\mathscr{W}_n(f_1, \ldots, f_n)$ is a separately continuous multilinear functional on $\bigtimes_1^n \mathscr{S}(\mathbb{R}^4)$. Thus, by the nuclear theorem (Theorem V.12), there is a distribution $\tilde{\mathscr{W}}_n$ in $\mathscr{S}'(\mathbb{R}^{4n})$ so that $\mathscr{W}_n(f_1, f_2, \ldots, f_n) = \tilde{\mathscr{W}}_n(f_1 f_2 \cdots f_n)$ if $f_i \in \mathscr{S}(\mathbb{R}^4)$. We denote $\tilde{\mathscr{W}}_n$ by $\mathscr{W}_n$ also.

From Properties 3 and 6 it follows that $\mathscr{W}_n$ has the invariance property:

$$\mathscr{W}_n(\langle a, \Lambda\rangle f_1, \ldots, \langle a, \Lambda\rangle f_n) = \mathscr{W}_n(f_1, \ldots, f_n)$$

for all $\langle a, \Lambda\rangle \in \mathscr{P}_+^\uparrow$. In particular,

$$\mathscr{W}_n(f_1(x_1 - a), f_2(x_2 - a), \ldots, f_n(x_n - a)) = \mathscr{W}_n(f_1, \ldots, f_n) \quad \text{(IX.35)}$$

By a simple analysis (see Problem 56), it follows from (IX.35) that there is a distribution $W_n \in \mathscr{S}'(\mathbb{R}^{4n-4})$ so that symbolically

$$\mathscr{W}_n(x_1, \ldots, x_n) = W_n(x_1 - x_2, x_2 - x_3, \ldots, x_{n-1} - x_n)$$

That is, for $f \in \mathscr{S}(\mathbb{R}^{4n})$,

$$\mathscr{W}_n(f) = \int_{\mathbb{R}_4} W_n(f_{(x)})\, dx$$

where

$$f_{(x)}(\xi_1, \ldots, \xi_{n-1}) = f(x, x - \xi_1, x - \xi_1 - \xi_2, \ldots, x - \xi_1 - \cdots - \xi_{n-1})$$

We have already introduced the notation V_+ for the forward light cone and $\bar{V}_+$ for the closed forward light cone. Define

$$V_+^{(n)} = \{\langle x_1, \ldots, x_n\rangle \in \mathbb{R}^{4n} \mid x_i \in V_+ \text{ for each } i\}$$

Note that $V_+^{(n)}$ and its closure $\bar{V}_+^{(n)}$ are cones. Let

$$\mathscr{T}_n = \mathbb{R}^{4n} - iV_+^{(n)}$$

We will call $\mathscr{T}_n$ the **forward tube**.

We are now ready to state and prove an important theorem about the Wightman distributions.

Theorem IX.32 For each $n \geq 1$, $\hat{W}_n$ has support in $-\bar{V}_+^{(n-1)}$ and W_n is the boundary value of a function analytic in the forward tube $\mathscr{T}_{n-1}$.

Proof Let k be given, $1 \leq k \leq n$, and let a be in $\mathbb{R}^4$. Then

$$\begin{aligned}
&\mathscr{W}_n(f_1(x_1) \cdots f_k(x_k) f_{k+1}(x_{k+1} - a) \cdots f_n(x_n - a)) \\
&\quad = (\psi_0, \varphi(f_1) \cdots \varphi(f_k) U(a) \varphi(f_{k+1}) \cdots \varphi(f_n)\psi_0) \\
&\quad = \int_{\mathbb{R}^4} e^{i\lambda \cdot \tilde{a}}\, d(\psi_1, E_\lambda \psi_2) \\
&\quad = \int_{\mathbb{R}^4} e^{i\tilde{\lambda} \cdot a}\, d(\psi_1, E_\lambda \psi_2) \\
&\quad = \int_{\mathbb{R}^4} e^{i\lambda \cdot a}\, d(\psi_1, E_{\tilde{\lambda}} \psi_2)
\end{aligned}$$

where $\psi_1 = \varphi(f_k)^* \cdots \varphi(f_1)^* \psi_0$ and $\psi_2 = \varphi(f_{k+1}) \cdots \varphi(f_n)\psi_0$. By Property 2, $d(\psi_1, E_\lambda \psi_2)$ has support in $\bar{V}_+$. Since $\lambda \mapsto \tilde{\lambda}$ takes $\bar{V}_+$ into itself, $d(\psi_1, E_{\tilde{\lambda}} \psi_2)$ also has support in $\bar{V}_+$. Now let

$$g(\xi_1, \ldots, \xi_{n-1}) = \prod_{j=2}^{n} f_j\left(-\sum_{i=1}^{j} \xi_i\right)$$

and suppose that $h_k \in \mathscr{S}(\mathbb{R}^4)$ is real-valued. In the following calculation we suppress the arguments $\xi_2, \ldots, \xi_{k-1}, \xi_{k+1}, \ldots, \xi_{n-1}$ of g.

$$\begin{aligned}
&\int_{\mathbb{R}^4} h_k(a) \mathscr{W}_n(f_1(x_1) \cdots f_k(x_k - a) \cdots f_n(x_n - a))\, da \qquad \text{(IX.36)} \\
&\quad = \int_{\mathbb{R}^4} \int_{\mathbb{R}^4} W_n(g(\xi_1 - x_1, \xi_k + a)) f_1(x_1) h_k(a)\, dx_1\, da \\
&\quad = W_n\left(\int_{\mathbb{R}^4} \int_{\mathbb{R}^4} g(\xi_1 - x_1, \xi_k + a) f_1(x_1) h_k(a)\, dx_1\, da\right) \\
&\quad = W_n(g * (f_1 \tilde{h}_k)) \\
&\quad = (2\pi)^{(n-1)/2} \hat{W}_n(\check{g} \check{f}_1 \hat{h}_k)
\end{aligned}$$

where $\tilde{h}_k(a) = h_k(-a)$. On the other hand,

$$\begin{aligned}
\text{(IX.36)} &= \int_{\mathbb{R}^4} h_k(a) \int_{\mathbb{R}^4} e^{i\tilde{\lambda} \cdot a}\, d(\psi_1, E_{\tilde{\lambda}} \psi_2)\, da \\
&= (2\pi)^{1/2} \int_{\mathbb{R}^4} \check{h}_k(\lambda)\, d(\psi_1, E_{\tilde{\lambda}} \psi_2)
\end{aligned}$$

Therefore $\hat{W}_n(\check{g}\check{f}_1\hat{h}_k) = 0$ if $(\operatorname{supp} \check{h}_k) \cap V_+ = \varnothing$. Since this is true for each k and since the set of finite linear combinations of such functions $\check{f}_1\check{g}$ is dense in $\mathscr{S}(\mathbb{R}^{4n-4})$, we conclude that the support of $\hat{W}_n$ is contained in $-V_+^{(n-1)}$. The conclusion of the theorem now follows from Theorem IX.16. ∎

Because the cone $V_+^{(n-1)}$ does not have a spherical base (if $n > 2$), we have used the generalization of Theorem X.16 given in Problem 23. The phrase "boundary value" in the statement of the theorem means boundary value in the sense of tempered distributions as explained in Section IX.3. Although we have not stated them explicitly, the estimates of Theorem IX.16 give corresponding estimates on the analytic continuation of the Wightman distributions.

An important use of the analyticity properties is to show that the Wightman functions obey certain symmetry relations. Here is a sketch of a typical argument. For simplicity of notation, we will pretend that the Wightman distributions are functions $W_n(\xi_1, \ldots, \xi_{n-1})$. The reader can easily supply the necessary test functions. Limits are always taken in the sense of $\mathscr{S}'(\mathbb{R}^{4n-4})$.

Because of Property 6,

$$W_n(z_1, \ldots, z_{n-1}) = W_n(\Lambda z_1, \ldots, \Lambda z_{n-1}) \tag{IX.37}$$

for all $z_j = \xi_i - i\eta_j$, $\eta_j \in V_+$ and $\Lambda \in \mathscr{L}_+^\uparrow$. Notice that the right-hand side of (IX.37) makes sense since $\Lambda\colon V_+ \to V_+$. Let $\mathscr{L}_+(\mathbb{C})$ denote the set of *complex* 4×4 matrices, Λ, of determinant one that satisfy $\Lambda z \cdot \widetilde{\Lambda z} = z \cdot \tilde{z}$. $\mathscr{L}_+(\mathbb{C})$ is a six-parameter complex manifold which contains the six-parameter real manifold $\mathscr{L}_+^\uparrow$. An elegant technical result, the Bargmann–Hall–Wightman theorem, states that W_n can be extended to be an analytic function on

$$\mathscr{T}_{n-1}^{e} = \{\langle \Lambda z_1, \ldots, \Lambda z_{n-1}\rangle \mid \langle z_1, \ldots, z_{n-1}\rangle \in \mathscr{T}_{n-1}, \Lambda \in \mathscr{L}_+(\mathbb{C})\}$$

so that (IX.37) still holds, but Λ is now allowed to range over $\mathscr{L}_+(\mathbb{C})$. $\mathscr{T}_{n-1}^{e}$ is called the **extended forward tube**. $\mathscr{T}_{n-1}^{e}$ contains certain real points called **Jost points**; in fact it can be shown that $\langle \xi_1, \ldots, \xi_{n-1}\rangle \in \mathscr{T}_{n-1}^{e} \cap \mathbb{R}^{4n-4}$ if and only if all vectors of the form $\zeta = \sum_{j=1}^{n-1} \lambda_j \xi_j$, with $\lambda_j \geq 0$ and $\sum \lambda_j > 0$, are spacelike, that is, $\xi \cdot \tilde{\xi} < 0$. Thus if $\langle x_1 - x_2, x_2 - x_3, \ldots, x_{n-1} - x_n\rangle$ is a Jost point, then

$$(x_i - x_j) \cdot \widetilde{(x_i - x_j)} < 0$$

for each i and j. By Property 7, it follows that

$$\mathscr{W}_n(x_1, \ldots, x_n) = \mathscr{W}_n(x_n, \ldots, x_1)$$

or

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(-\xi_{n-1}, \ldots, -\xi_1) \tag{IX.38}$$

when $\langle \xi_1, \ldots, \xi_{n-1}\rangle$ is a Jost point. Since $-I \in \mathscr{L}_+(\mathbb{C})$, (IX.37) and (IX.38) together imply that

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(\xi_{n-1}, \ldots, \xi_1) \tag{IX.39}$$

Since W_n is analytic in $\mathscr{T}_{n-1}^{e}$ and (IX.39) holds on an open subset of a $\mathbb{R}^{4n-4}$-dimensional subspace, (IX.39) holds throughout $\mathscr{T}_{n-1}^{e}$, i.e.

$$W_n(z_1, \ldots, z_{n-1}) = W_n(z_{n-1}, \ldots, z_1) \tag{IX.40}$$

for $z = \langle z_1, \ldots, z_{n-1}\rangle \in \mathscr{T}_{n-1}^{e}$. If $z_j = \xi_j - i\eta_j$ with $\eta_j \in V_+$, then by Theorem IX.16, $W_n(z_1, \ldots, z_{n-1})$ converges to $W_n(\xi_1, \ldots, \xi_{n-1})$ and $W_n(z_{n-1}, \ldots, z_1)$ converges to $W_n(\xi_{n-1}, \ldots, \xi_1)$ in the sense of distributions as $\eta \downarrow 0$. Thus (IX.39) holds for all $\langle \xi_1, \ldots, \xi_{n-1}\rangle \in \mathbb{R}^{4n-4}$ and it follows that

$$\mathscr{W}_n(x_1, \ldots, x_n) = \mathscr{W}_n(-x_n, \ldots, -x_1) \tag{IX.41}$$

for all $\langle x_1, \ldots, x_n\rangle \in \mathbb{R}^{4n}$. Now, define an operator Θ by

$$\Theta\varphi(f_1) \cdots \varphi(f_{n+1})\psi_0 = \varphi(\tilde{\bar{f}}_1) \cdots \varphi(\tilde{\bar{f}}_{n+1})\psi_0$$

and extend Θ to D_0 by real linearity. By (IX.41), Θ is norm-preserving and thus well defined. It is easily checked that $\Theta(\psi_1 + \psi_2) = \Theta(\psi_1) + \Theta(\psi_2)$ and $\Theta(c\psi) = \bar{c}\Theta\psi$; such an operator is called **antilinear**. By Property 8, D_0 is dense in $\mathscr{H}$. So, since $\Theta^2 = I$, Θ extends uniquely to an antiunitary operator on $\mathscr{H}$ which satisfies

$$\Theta\varphi(f)\Theta^{-1} = \varphi(\tilde{\bar{f}}) \qquad \text{for all } f \in \mathscr{S}(\mathbb{R}^4)$$

The existence of such a Θ is just the celebrated **PCT theorem** for the case of a Hermitian scalar field theory.

We remark that some care is needed in using these analyticity arguments. For example, (IX.38) and the analyticity imply that

$$W_n(z_1, \ldots, z_{n-1}) = W_n(-z_{n-1}, \ldots, -z_1) \tag{IX.42}$$

throughout the extended forward tube. But, we *cannot* conclude from this that

$$W_n(\xi_1, \ldots, \xi_{n-1}) = W_n(-\xi_{n-1}, \ldots, -\xi_1) \tag{IX.43}$$

for $\langle \xi_1, \ldots, \xi_{n-1}\rangle \in \mathbb{R}^{4n-4}$ by taking boundary values. $W_n(\xi_1, \ldots, \xi_{n-1})$ is the boundary value of $W_n(z_1, \ldots, z_{n-1})$ as $z_j \to x_j$ in the forward tube. But, if $\eta_j \in V_+$ then $-\eta_j \notin V_+$ so $\langle -z_{n-1}, \ldots, -z_1\rangle$ is not in the forward tube. Thus the limit of $W_n(-z_{n-1}, \ldots, -z_1)$ in the sense of $\mathscr{S}'(\mathbb{R}^{4n-4})$ may have nothing to do with $W_n(-\xi_{n-1}, \ldots, -\xi_1)$.

The Wightman axioms place fairly strong restrictions on the distributions W_n. As a final illustration of this fact we will use Fourier transform methods to derive the Källen–Lehmann representation of the two-point function W_2. In order to do this we need a theorem about Lorentz invariant measures. For each $m \geq 0$, let $H_m = \{x \in \mathbb{R}^4 \,|\, x \cdot \tilde{x} = m^2,\ x_0 > 0\}$. The sets H_m, which are called **mass hyperboloids**, are invariant under $L_+^\uparrow$. Let j_m be the homeomorphism of H_m onto $\mathbb{R}^3$ (or in the case $m = 0$ onto $\mathbb{R}^3 \backslash 0$) given by $j_m : \langle x_0, x_1, x_2, x_3 \rangle \mapsto \langle x_1, x_2, x_3 \rangle = \mathbf{x}$. Define a measure Ω_m on H_m by setting

$$\Omega_m(E) = \int_{j_m(E)} \frac{d^3x}{\sqrt{m^2 + |\mathbf{x}|^2}}$$

for any measurable set $E \subset H_m$. The measure Ω_m can easily be seen to be $L_+^\uparrow$-invariant. In fact, up to a constant multiple, Ω_m is the only $L_+^\uparrow$-invariant measure on H_m (see the Appendix). Furthermore, every polynomially bounded $L_+^\uparrow$-invariant measure on $\bar{V}_+$ is the sum of a multiple of δ and an integral of the measures Ω_m. We state this fact as a theorem.

Theorem IX.33 Let μ be a polynomially bounded measure with support in $\bar{V}_+$. If μ is $L_+^\uparrow$-invariant, there exists a polynomially bounded measure ρ on $[0, \infty)$ and a constant c so that

$$\int_{\mathbb{R}^4} f \, d\mu = cf(0) + \int_0^\infty \left(\int_{H_m} f \, d\Omega_m \right) d\rho(m)$$

for all $f \in \mathscr{S}(\mathbb{R}^4)$.

Proof See the Appendix to this section.

Theorem IX.34 (Källen–Lehmann representation) Let W_2 be the two-point function of a field theory satisfying the Wightman axioms and the additional condition that $(\psi_0, \varphi(f)\psi_0) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$. Then there exists a polynomially bounded positive measure on $[0, \infty)$ so that for all $f \in \mathscr{S}(\mathbb{R}^4)$,

$$W_2(f) = \int_0^\infty \left(\int_{H_m} \hat{f} \, d\Omega_m \right) d\rho(m)$$

Symbolically,

$$W_2(x) = \int_0^\infty \frac{1}{i} \Delta_+(x; m^2) \, d\rho(m)$$

where

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3} \int_{\mathbb{R}^3} \frac{\exp(-ix_0\sqrt{m^2 + \mathbf{k}^2} + i\mathbf{x} \cdot \mathbf{k})}{\sqrt{m^2 + \mathbf{k}^2}} \, d^3\mathbf{k}$$

Proof Let $f \in \mathscr{S}(\mathbb{R}^4)$. Then

$$\begin{aligned} \iint \overline{f(x)} f(y) W_2(x - y) \, dx \, dy &= (\psi_0, \varphi(\bar{f})\varphi(f)\psi_0) \\ &= \|\varphi(f)\psi_0\|^2 \geq 0 \end{aligned}$$

Thus W_2 is a distribution of positive type. By the Bochner–Schwartz theorem, $\check{W}_2$ is a polynomially bounded measure and by Theorem IX.27 the support of $\check{W}_2$ is contained in $\bar{V}_+$. Since $\mathscr{W}_2$ is $\mathscr{L}_+^\uparrow$-invariant, W_2 is invariant and the reader can easily check that this implies that $\check{W}_2$ is $\mathscr{L}_+^\uparrow$-invariant. Thus $\check{W}_2$ satisfies all the hypotheses of Theorem IX.33, so

$$W_2(f) = c\hat{f}(0) + \int_0^\infty \left(\int_{H_m} \hat{f} \, d\Omega_m \right) d\rho(m)$$

for some polynomially bounded measure ρ on $[0, \infty)$ and some constant c.

To conclude the proof we will use the hypothesis that $(\psi_0, \varphi(f)\psi_0) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$ to prove that $c = 0$. Let $g \in \mathscr{S}(\mathbb{R}^4)$ and define $G(a) = (\varphi(g)\psi_0, U(-a, I)\varphi(g)\psi_0)$. Then,

$$\begin{aligned} G(a) &= (\psi_0, \varphi(\bar{g})\varphi(g_{-a}(x))\psi_0) = (W_2 * g_{-a})(\bar{g}) \\ &= (W_2 * g)(\bar{g}_a) = (W_2 * g * \tilde{\bar{g}})(a) \end{aligned}$$

Therefore, $\check{G}$ is the measure $|\check{g}(k)|^2 \check{W}_2$. But

$$\begin{aligned} G(a) &= \int e^{-ia \cdot \lambda} \, d(\varphi(g)\psi_0, E_\lambda \varphi(g)\psi_0) \\ &= \int e^{-ia \cdot \lambda} \, d(\varphi(g)\psi_0, E_{\tilde{\lambda}} \varphi(g)\psi_0) \end{aligned}$$

so $\check{G}$ is also the measure $(2\pi)^2 \, d(\varphi(g)\psi_0, E_{\tilde{\lambda}}\varphi(g)\psi_0)$. Since the vacuum is unique (Property 3), the mass of $d(\varphi(g)\psi_0, E_{\tilde{\lambda}}\varphi(g)\psi_0)$ at the origin is $|(\psi_0, \varphi(g)\psi_0)|^2$ which equals zero by hypothesis. Thus $|\check{g}(k)|^2 \check{W}_2$ has no mass at the origin. Since this is true for all $g \in \mathscr{S}(\mathbb{R}^4)$, we conclude that $c = 0$. ∎

We remark that Theorem IX.32 can be combined with microscopic causality to prove analyticity properties for certain distributions arising from commutators of the field. For example, if we define

$$C_2(y - x) = (\psi_0, \varphi(x)\varphi(y)\psi_0) - (\psi_0, \varphi(y)\varphi(x)\psi_0)$$

then by Property 7, C_2 has support in $\bar{V}_+ \cup (-\bar{V}_+)$. Such a distribution can be written $C_2 = R_2 + A_2$ where supp $R_2 \subset \bar{V}_+$ and supp $A_2 \subset -\bar{V}_+$; see Problem 56. R_2 is obviously determined up to a distribution with support at the origin. Since supp $R_2 \subset \bar{V}_+$, the Fourier transform of R_2 is analytic in the tube $\mathbb{R}^4 - iV_+$. For R_2 this can be seen directly from the Källen–Lehmann representation. For a general model, one would like to prove that the higher order commutators C_n can be written as a sum of distributions with supports in cones. The corresponding retarded functions R_n would then have Fourier transforms which are the boundary values of analytic functions. The analyticity properties of the $\hat{R}_n$ are related to the analyticity of the scattering amptitude.

Appendix to IX.8 Lorentz invariant measures

The purpose of this appendix is to prove the facts about Lorentz invariant measures used in Section IX.8. In particular we will prove Theorem IX.33. First we need some general results about measures on product spaces.

Theorem IX.35 (a) Let X be a locally compact space and let $\{T_\alpha\}_{\alpha \in A}$ be a family of homeomorphisms of X into itself. Suppose that there is precisely one (up to constant multiples) Baire measure μ invariant under all the T_α. Let Y be another locally compact space and define $T_\alpha \times I$ by $T_\alpha \times I: \langle x, y\rangle \mapsto \langle T_\alpha x, y\rangle$ for all $\langle x, y\rangle \in X \times Y$. Then any Baire measure ρ on $X \times Y$ invariant under all the maps $T_\alpha \times I$ is of the form $\rho = \mu \otimes \nu$ for some Baire measure ν on Y.

(b) If X and Y are locally compact spaces and $\mu_1 \otimes \nu_1 = \mu_2 \otimes \nu_2$ for nonzero measures $\mu_1, \mu_2, \nu_1, \nu_2$, then $d\mu_1 = c\, d\mu_2$ and $d\nu_1 = c^{-1}\, d\nu_2$.

Proof Let ρ be invariant under the $T_\alpha \times I$ and choose $f \in \kappa(Y)$, the continuous functions of compact support, with $f \geq 0$. Let ρ_f be the map from $\kappa(X)$ to $\mathbb{R}$ defined by $\rho_f: g \mapsto \rho(g \otimes f)$. Since ρ_f is a positive linear form on $\kappa(X)$, it is a Baire measure. In addition ρ_f is invariant under the maps T_α since ρ is invariant under the maps $T_\alpha \times I$, so by hypothesis $\rho_f = c_f \mu$ for some constant c_f. Since, by hypothesis $\mu \neq 0$, we can find a positive function $g \in \kappa(X)$ so that $\mu(g) > 0$. Then $c_f = \rho(g \otimes f)/\mu(g)$ is a positive linear form on $\kappa(Y)$ so $c_f = \nu(f)$ for some Baire measure ν, i.e. $\rho = \mu \otimes \nu$. This proves (a).

To prove (b) we first observe that μ_1 and μ_2 and also ν_1 and ν_2 must have the same sets of zero measure. Let f and g be the characteristic functions of sets E and F in X and Y respectively where $\mu_1(f) \neq 0 \neq \nu_2(g)$. Then $\mu_2(E)/\mu_1(E) = \nu_1(F)/\nu_2(F)$ from which (b) immediately follows. ∎

We will need some information about measures on $\mathbb{R}^n$ and $\mathbb{R}^+$.

Theorem IX.36

(a) Constant multiples of Lebesgue measure are the only translation-invariant Baire measures on $\mathbb{R}^n$.

(b) The only Baire measures on $\mathbb{R}^+ = (0, \infty)$ that are invariant under all the transformations $T_a: x \mapsto e^a x$ (all $a \in \mathbb{R}$) are constant multiples of the measure dx/x.

Proof We begin by proving (a) for the case $n = 1$. We need only show that if μ is translation invariant and $\mu([0, 1]) = 1$, then μ is Lebesgue measure. Since $\mu(\{x\})$ is independent of x and $[0, 1]$ contains infinitely many points, we must have $\mu(\{x\}) = 0$. Thus $\mu([0, 1)) = 1$. Since $[0, 1)$ is a union of n translates of $[0, 1/n)$, we have $\mu([0, 1/n)) = 1/n$ and it easily follows from this that $\mu([0, r)) = r$ for any positive rational number r. Translation invariance then implies that if a and b are rationals and $a < b$, then $\mu((a, b)) = b - a$. But since μ is a Baire measure, it is regular which implies $\mu((a, b)) = b - a$ for all $a < b$. Since μ is determined by its values on finite open intervals, μ must be Lebesgue measure.

We now complete the proof of (a) by induction. Suppose that the only translation invariant measures in $\mathbb{R}^k$ are multiples of $d^k x$ and let ρ be a translation invariant measure on $\mathbb{R}^{k+1} = \mathbb{R}^k \times \mathbb{R}$. Since ρ is invariant under the subgroup of translations of the form $T \times I$ it is of the form $d^k x \otimes d\nu$ by Theorem IX.35a. Since ρ is also invariant under the subgroup of the form $I \times T$ it is of the form $d\mu \otimes dx$. Thus, by Theorem IX.35b, $\rho = c\, d^k x \otimes dx = c\, d^{k+1} x$.

(b) follows from (a) since $\ln: x \to \ln(x)$ is a homeomorphism of $\mathbb{R}^+$ onto $\mathbb{R}$ under which T_a goes over into translation by a. ∎

We are now ready to examine Lorentz invariant measures on $\bar{V}_+$; i.e. polynomially bounded measures with support in $\bar{V}_+$ which are invariant under $\mathscr{L}_+^\uparrow$. $\bar{V}_+$ can be written $\bar{V}_+ = \{0\} \cup (\bigcup_{m=0}^\infty H_m)$. Further, the set $\{0\}$ and each of the H_m are taken into themselves by $\mathscr{L}_+^\uparrow$. First we will examine H_m and show that it has only one invariant measure Ω_m (defined in Section 8). Then we will prove Theorem IX.33 which says that any Lorentz

invariant measure on $\bar{V}_+$ can be obtained by "adding up" a delta function at $\langle 0, 0, 0, 0\rangle$ and these invariant measures on the H_m. Although there will be many changes of variable in the following proofs, the idea of all of them is the same: to homeomorphically map the space one is interested in onto a product space $X \times Y$, to analyze the invariant measures on X and Y by Theorem IX.36, and then to determine the invariant measures on $X \times Y$ (and thus on the original space) by using Theorem IX.35.

Lemma The measure $\Omega_m(\cdot)$ on H_m is invariant under $\mathscr{L}_+^\uparrow$.

Proof One straightforward way of seeing that Ω_m is Lorentz invariant is to compute the action of any $\Lambda \in \mathscr{L}_+^\uparrow$ on H_m, proving that the Jacobians work out to keep Ω_m invariant. A more instructive proof first notes that d^4x is $\mathscr{L}_+^\uparrow$-invariant since $\Lambda \in \mathscr{L}_+^\uparrow$ implies $\det \Lambda = 1$. Let $f \in C_0^\infty(0, \infty)$; then since V_+ is $\mathscr{L}_+^\uparrow$-invariant, the measure $f(x \cdot \tilde{x})\chi\, d^4x$ is $\mathscr{L}_+^\uparrow$-invariant where χ is the characteristic function of V_+. Now map V_+ homeomorphically onto $\mathbb{R}^3 \times \mathbb{R}^+$ by h: $\langle x_0, \mathbf{x}\rangle \mapsto \langle \mathbf{x}, y\rangle$ where $y = x \cdot \tilde{x}$. Then $\partial y/\partial x_0 = 2x_0$ so

$$d^4x = \frac{d^3\mathbf{x}\, dy}{2\sqrt{m^2 + x^2}}$$

Thus, the measure

$$\Omega^f(E) = \int_{h[E]} \frac{f(y)\, d^3\mathbf{x}\, dy}{\sqrt{m^2 + \mathbf{x}^2}}$$

is $\mathscr{L}_+^\uparrow$-invariant. If $f_n(y)$ is a sequence in $C_0^\infty(0, \infty)$ converging to $\delta(y - m^2)$, $m > 0$, then Ω^{f_n} converges to Ω_m in $\mathscr{S}'(\mathbb{R}^4)$ and thus Ω_m is $\mathscr{L}_+^\uparrow$-invariant in the sense that $\Omega_m(g(x)) = \Omega_m(g(\Lambda x))$ for all $g \in \mathscr{S}(\mathbb{R}^4)$, $\Lambda \in \mathscr{L}_+^\uparrow$. By a simple argument, this implies $\Omega_m(E) = \Omega_m(\Lambda E)$ for $m > 0$. Since $\Omega_m \to \Omega_0$ in $\mathscr{S}'(\mathbb{R}^4)$ as $m \downarrow 0$ we have also proven the case where $m = 0$. ∎

Because of the way $d\Omega_m$ was constructed in the above proof, some physics literature denotes $d\Omega_m$ by $\delta(x^2 - m^2)\, d^4x$ or even as $\delta(x^2 - m^2)$.

Theorem IX.37 Ω_m is the unique $\mathscr{L}_+^\uparrow$-invariant measure on H_m, $m \geq 0$.

Proof We begin by choosing a new coordinate system for $\mathbb{R}^4$ by letting $\tau = 2^{-1/2}(x_0 - x_3)$, $z = 2^{-1/2}(x_0 + x_3)$, and $\mathbf{x} = \langle x_1, x_2\rangle \in \mathbb{R}^2$. In this new coordinate system the Lorentz inner product is

$$x \cdot \tilde{x} = 2z\tau - \mathbf{x} \cdot \mathbf{x}$$

On any H_m, $m > 0$, we can use τ and $\mathbf{x}$ as coordinates since $z = (2\tau)^{-1}(\mathbf{x} \cdot \mathbf{x} + m^2)$. Notice that if $x \in H_m$ and $m > 0$, then both z and τ are in $(0, \infty)$.

Let ρ be an invariant measure on H_m, $m > 0$, and let s be the homeomorphism of H_m onto $\mathbb{R}^2 \times \mathbb{R}^+$ given by $x \mapsto \langle \mathbf{x}, \tau\rangle$. Let L_a, $a \in \mathbb{R}$, be the linear transformation on $\mathbb{R}^4$ given by $\tau \to e^a\tau$, $z \to e^{-a}z$, $\mathbf{x} \to \mathbf{x}$. Since L_a preserves the form $2z\tau - \mathbf{x} \cdot \mathbf{x}$, $\det L_a = 1$ and L_a: $V_+ \to V_+$, it is a Lorentz transformation and sL_as^{-1}: $\langle \mathbf{x}, \tau\rangle \mapsto \langle \mathbf{x}, e^a\tau\rangle$. Since $s(d\rho)$ is a measure on $\mathbb{R}^2 \times \mathbb{R}^+$ invariant under sL_as^{-1} for all $a \in \mathbb{R}$, we conclude from Theorem IX.36b and Theorem IX.35a that $s(d\rho) = d\mu(\mathbf{x}) \otimes d\tau/\tau$.

Now, let $T_\mathbf{b}$: $\mathbb{R}^4 \to \mathbb{R}^4$, $\mathbf{b} \in \mathbb{R}^2$ be the transformation

$$T_\mathbf{b}\colon \langle \tau, z, \mathbf{x}\rangle \mapsto \langle \tau, z + \mathbf{b} \cdot \mathbf{x} + \tfrac{1}{2}|\mathbf{b}|^2\tau, \mathbf{x} + \tau\mathbf{b}\rangle$$

A short calculation shows that $T_\mathbf{b} \in L_+^\uparrow$. It is clear that $sT_\mathbf{b}s^{-1}$: $\langle \mathbf{x}, \tau\rangle \mapsto \langle \mathbf{x} + \tau\mathbf{b}, \tau\rangle$. Let t: $\langle \mathbf{x}, \tau\rangle \mapsto \langle \mathbf{x}/\tau, \tau\rangle$. Then t: $\mathbb{R}^2 \times \mathbb{R}^+ \mapsto \mathbb{R}^2 \times \mathbb{R}^+$ and $tsT_\mathbf{b}s^{-1}t^{-1}$: $\langle \mathbf{x}, \tau\rangle \mapsto \langle \mathbf{x} + \mathbf{b}, \tau\rangle$. Using Theorems IX.36a and IX.35a we conclude that $ts(d\rho) = d^2x \otimes dv(\tau)$; i.e. $s(d\rho) = d^2x \otimes dv(\tau)/\tau^2$.

Since $s(d\rho) = d\mu \otimes d\tau/\tau$ and $s(d\rho) = d^2x \otimes dv(\tau)/\tau^2$, we conclude by Theorem IX.35b that $s(d\rho) = c\, d^2x \otimes d\tau/\tau$. Since s sets up a one-to-one correspondence between the measures on H_m and the measures on $\mathbb{R}^2 \times \mathbb{R}^+$, it follows that there is at most one (up to constant multiples) measure on H_m invariant under $\mathscr{L}_+^\uparrow$. By the lemma we know there is at least one such measure, so there is exactly one.

The proof for the case $m = 0$ is similar. We only note first that the set $\{x \mid \tau = 0\}$ must have ρ-measure zero. ∎

Proof of Theorem IX.33 Let μ be a polynomially bounded measure invariant under $\mathscr{L}_+^\uparrow$, with support in V_+. Let χ_0 be the characteristic function of H_0, χ the characteristic function of $\bigcup_{m>0} H_m$. Then $\chi_0\mu$ is $\mathscr{L}_+^\uparrow$-invariant, so $\chi_0\mu = e\Omega_0$, i.e. $\mu = \mu(\{0\})\delta_0 + e\Omega_0 + \chi\mu$. Let j be the homeomorphism of $\bigcup_{m>0} H_m$ defined by j: $\langle x_0, \mathbf{x}\rangle \mapsto \langle \mathbf{x}/x \cdot \tilde{x}, x \cdot \tilde{x}\rangle$. For each $\Lambda \in L_+^\uparrow$, $j\Lambda j^{-1}$ acts on $\mathbb{R}^3 \times \mathbb{R}^+$ by a product action $\Lambda_s \times I$. The measure $j(\chi\mu)$ is invariant under the maps $\Lambda_s \times I$. By Theorem IX.37 there is a unique measure Ω on $\mathbb{R}^3$ invariant under all Λ_s and $\Omega = c_m j(\Omega_m)$ for each m. By Theorem IX.35a, $h(\chi\mu) = \Omega \otimes \tilde{\rho}$ for some Baire measure $\tilde{\rho}$ on $(0, \infty)$. That is, for $f \in \mathscr{S}(\mathbb{R}^4)$

$$\int_{V_+} f(x)\, d\mu(x) = \int_{\mathbb{R}^+} \left(\int_{\mathbb{R}^3} f(j^{-1}(x))\, d\Omega \right) d\tilde{\rho}(m)$$

$$= \int_{\mathbb{R}^+} \left(\int_{H_m} f(x) c_m\, d\Omega_m \right) d\tilde{\rho}(m)$$

Now define ρ on $[0, \infty)$ by $\rho = c_m \tilde{\rho} + e\delta_0$. Then,

$$\int_{\mathbb{R}^4} f(x)\, d\mu(x) = \mu(\{0\}) f(0) + \int_{m \geq 0} \left(\int f(x)\, d\Omega_m \right) d\rho(m)$$

The fact that ρ is polynomially bounded follows from the polynomial boundedness of μ. ∎

IX.9 Restriction to submanifolds

Let M be a hyperplane or a compact submanifold of $\mathbb{R}^n$ of dimension $n-1$ or less. In this section we consider the problem of which $f \in L^2(\mathbb{R}^n)$ can be restricted in a natural way to M. Since M has Lebesgue measure zero in $\mathbb{R}^n$, we will not be able to restrict every f to M. We only expect to be able to restrict those f such that there is a distinguished element in the equivalence class of f which is suitably smooth. For example, an $f \in \mathscr{S}(\mathbb{R}^n)$ has a natural restriction $T_M f$ given by merely taking the values of f on M. The idea of our approach is to find a Banach space B with $\mathscr{S}(\mathbb{R}^n) \subset B \subset L^2(\mathbb{R}^n)$ so that for $f \in \mathscr{S}(\mathbb{R}^n)$, $\|T_M f\|_{L^2(M)} \leq C\|f\|_B$. If $\mathscr{S}(\mathbb{R}^n)$ is dense in B, then we can use the B.L.T. theorem to extend T_M to all of B. A second approach to the restriction problem is discussed in the Notes to Section IX.10.

What shall we take for the Banach space B? Our experience suggests that smoothness conditions on f are equivalent to decay bounds of $\hat{f}$ so it is natural to try to use the Sobolev spaces W_m. For notational convenience we introduce the **weighted L^2 space** L^2_m. We say $f \in L^2_m(\mathbb{R}^n)$ if and only if $\hat{f} \in W_m$, i.e., if and only if

$$\int_{\mathbb{R}^n} (1 + |x|^2)^m |f(x)|^2\, dx < \infty$$

There is a natural question which is dual to the restriction problem that we have posed. Namely, given $f \in L^2(M)$, we can associate f with a tempered distribution $T_M^* f$ on $\mathbb{R}^n$ with the action $T_M^* f\colon \varphi \to \int_M f(x)\varphi(x)\, d\omega$ where ω is the natural measure (see below) on M. What are the growth properties of $\mathscr{F}_M f \equiv \widehat{T_M^* f}$? We begin by solving these two problems for hyperplanes.

Theorem IX.38 Let $f \in \mathscr{S}(\mathbb{R}^n)$ and suppose that M is a plane in $\mathbb{R}^n$ of codimension k, $1 \leq k \leq n-1$.

(a) Let $T_M f$ be the restriction of f to M. Then there is a constant C (independent of f) so that $\|T_M f\|_{L^2(M)} \leq C\|f\|_{W_m}$ for all $m > k - \frac{1}{2}$. Thus T_M extends uniquely to a bounded map of W_m into $L^2(M)$.

(b) Let $d_M x$ be Lebesgue measure on M (defined for example by translating M to the origin and choosing an orthonormal basis) and let $f \in L^2(M, d_M x)$. Define

$$(\mathscr{F}_M f)(\lambda_1, \ldots, \lambda_n) = \frac{1}{(2\pi)^{n/2}} \int_M e^{-ix \cdot \lambda} f(x)\, d_M x \qquad \text{(IX.44)}$$

Then $\mathscr{F}_M f$ is the Fourier transform of f regarded as a tempered distribution and $\mathscr{F}_M f \in L^2_m(\mathbb{R}^n)$ for all $m < -k + \frac{1}{2}$.

Proof We will give a proof for the case $n = 2$, $k = 1$. The proof of the general case uses the same ideas and is left as an exercise (Problem 57). Since both the hypotheses and conclusions are invariant under translations and rotations of M, we may assume that $M = \{\langle x_1, 0\rangle \mid x_1 \in \mathbb{R}\}$.

To prove (a), let $m > \frac{1}{2}$. Then

$$|f(x_1, 0)| \leq \int \left| \int \frac{e^{ix_1\lambda_1}}{2\pi} \hat{f}(\lambda_1, \lambda_2)\, d\lambda_1 \right| d\lambda_2$$

$$\leq \left(\int \frac{d\lambda_2}{(1 + \lambda_2^2)^m} \right)^{1/2} \left(\int (1 + |\lambda_2|^2)^m \left| \int e^{ix_1\lambda_1} \hat{f}(\lambda_1, \lambda_2) \frac{d\lambda_1}{2\pi} \right|^2 d\lambda_2 \right)^{1/2}$$

so, by the Plancherel theorem in one variable,

$$\int |f(x_1, 0)|^2\, dx_1 \leq C \int \left(\int (1 + |\lambda_2|^2)^m \left| \int e^{ix_1\lambda_1} \hat{f}(\lambda_1, \lambda_2) \frac{d\lambda_1}{\sqrt{2\pi}} \right|^2 d\lambda_2 \right) dx_1$$

$$= C \int (1 + |\lambda_2|^2)^m |\hat{f}(\lambda_1, \lambda_2)|^2\, d\lambda_1\, d\lambda_2$$

$$\leq C \int (1 + |\lambda_1|^2 + |\lambda_2|^2)^m |\hat{f}(\lambda_1, \lambda_2)|^2\, d\lambda_1\, d\lambda_2$$

$$= C\|f\|_{W_m}$$

Thus, the restriction map $T_M f = f(\cdot, 0)$ extends to a bounded map of W_m into $L^2(M)$.

Now, suppose that $g \in L^2(M, d_M x) = L^2(\mathbb{R})$. Let χ_n be the characteristic function of $(-n, n)$. Then $\chi_n(x_1) g(x_1) \delta(x_2)$ is a distribution on $\mathbb{R}^2$ with compact support, so by Theorem IX.5,

$$\widehat{\chi_n g \delta}(\lambda_1, \lambda_2) = \frac{1}{2\pi} \int e^{-i\lambda_1 x_1} \chi_n(x_1) g(x_1)\, dx_1$$

If $\varphi \in \mathscr{S}(\mathbb{R}^2)$, then

$$\iint \left(\frac{1}{2\pi}\int e^{-i\lambda_1 x_1}\chi_n(x_1)g(x_1)\,dx_1\right)\varphi(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2$$

$$\longrightarrow \iint \left(\frac{1}{2\pi}\int e^{-i\lambda_1 x_1}g(x_1)\,dx_1\right)\varphi(\lambda_1,\lambda_2)\,d\lambda_1\,d\lambda_2$$

so, since $\chi_n g \to g$ weakly and the Fourier transform is weakly continuous, $(2\pi)^{-1}\int e^{-i\lambda_1 x_1}g(x_1)\,dx_1$ is just the Fourier transform of $g(x_1)\delta(x_2)$ as a distribution on $\mathbb{R}^2$. To complete the proof, we let $m < -\frac{1}{2}$. Then

$$\iint (1+|\lambda_1|^2+|\lambda_2|^2)^m |(\mathscr{F}_{\mathbb{R}} g)(\lambda_1,\lambda_2)|^2\,d\lambda_1\,d\lambda_2$$

$$\leq (2\pi)^{-1}\iint (1+|\lambda_2|^2)^m |\hat{g}(\lambda_1)|^2\,d\lambda_1\,d\lambda_2$$

$$\leq (2\pi)^{-1}\left(\int (1+|\lambda_2|^2)^m\,d\lambda_2\right)\|g\|^2_{L^2(\mathbb{R})}$$

so $\mathscr{F}_{\mathbb{R}} g \in L^2_m(\mathbb{R}^2)$. ∎

We turn now to the case where M is a compact submanifold.

Definition A **hypersurface** M in $\mathbb{R}^n$ is a set of points with the following property: there is a real-valued C^∞ function F on $\mathbb{R}^n$ so that $M = \{x \mid F(x) = 0\}$ and so that $\nabla F = \langle \partial F/\partial x_1, \ldots, \partial F/\partial x_n\rangle \neq 0$ at each $x \in M$. More generally, a **regularly imbedded submanifold of codimension k** is the set of points where k real-valued C^∞ functions vanish with the additional property that the Jacobian matrix $\{\partial F_i/\partial x_j\}_{1\leq i\leq k,\ 1\leq j\leq n}$ have rank k at each point in M.

For simplicity of notation we will discuss only the case of codimension one. Once F is given, the hypersurface (and more generally, regularly imbedded submanifolds) carries a natural measure. We will describe it in a neighborhood of $x \in M$. Since $\nabla F(x) \neq 0$, $\partial F/\partial x_\ell \neq 0$ for some ℓ. By the implicit function theorem of advanced calculus we can find a neighborhood N of x and a smooth function h_ℓ on $\mathbb{R}^{n-1}$ so that $x_\ell = h_\ell(x_1, \ldots, \hat{x}_\ell, \ldots, x_n)$ for all $\langle x_1, \ldots, x_n\rangle \in N \cap M$, where $\langle x_1, \ldots, \hat{x}_\ell, \ldots, x_n\rangle$ means omit the ℓth coordinate. For each $S \subset (N \cap M)$, we define

$$\omega_N(S) = \int_{h_\ell^{-1}(S)} \frac{dx_1 \cdots d\hat{x}_\ell \cdots dx_n}{|\partial F/\partial x_\ell|}$$

Then by the chain rule and the Jacobian formula for change of variables the measure ω_N is independent of which ℓ with $\partial F/\partial x_\ell \neq 0$ we chose. By piecing the measures ω_N together we can get a natural measure on all of M. The reader can check that the natural measure on S^{n-1} (the surface of the unit ball in $\mathbb{R}^n$) is just the usual spherical measure if

$$F(x_1, \ldots, x_n) = \frac{1}{2}\left(\sum_{i=1}^n x_i^2 - 1\right)$$

We remark that the measure we have constructed above is F dependent. But, if M is compact, then any two such measures are absolutely continuous with respect to one another and their Radon–Nikodym derivatives are bounded from above and below by positive constants. Thus the corresponding L^2-spaces on M are the same in the sense that their norms are equivalent. We warn the reader that there is a natural measure on M which can be constructed geometrically but which may differ from the ones we have constructed; see the Notes. If M is compact, then the L^2 space of this geometric measure is the same as the L^2 spaces of the F-dependent measures.

Theorem IX.39 Let M be a regularly imbedded compact submanifold in $\mathbb{R}^n$ of codimension k given by k C^∞ functions $F_1, \ldots, F_k$. We denote by ω the natural induced measure on M. Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$.

(a) Let $T_M f$ be the restriction of f to M. Then for all $m > k - \frac{1}{2}$, there is a constant C (independent of f) so that $\|T_M f\|_{L^2(M,\,d\omega)} \leq C\|f\|_{W_m}$ so T_M extends uniquely to a bounded map of W_m into $L^2(M, d\omega)$.

(b) Let $f \in L^2(M, d\omega)$ and define

$$(\mathscr{F}_M f)(\lambda_1, \ldots, \lambda_n) = \frac{1}{(2\pi)^{n/2}}\int_M e^{-ix\cdot\lambda} f(x)\,d\omega \qquad \text{(IX.45)}$$

Then $\mathscr{F}_M f$ is the Fourier transform of the tempered distribution on $\mathbb{R}^n$ associated to f, $\mathscr{F}_M f$ is in $C^\infty(\mathbb{R}^n)$, and $\mathscr{F}_M f \in L^2_m(\mathbb{R}^n)$ for all $m < -k + \frac{1}{2}$.

Proof As before, we only give the proof in the case of codimension one. The proof consists of essentially the same computations as in Theorem IX.38, except that we must break the manifold up into a finite number of pieces each of which we flatten out so we can use the Plancherel theorem. In this way we will prove (b). We then avoid the computation in (a) by a duality argument.

Let $f \in L^2(M, d\omega)$. Then f can be associated with a distribution of compact support under the action

$$\varphi \mapsto \int_M f(x)\varphi(x)\, d\omega$$

Since this distribution has compact support, Theorem IX.5 implies that the formula (IX.45) gives its Fourier transform. $\mathscr{F}_M f$ is in C^∞ by the Paley–Wiener theorem for distributions.

By using the implicit function theorem and the compactness of M, we can find a decomposition of M into disjoint measurable sets $S_1, \ldots, S_N$:

$$S_j = \{\langle x_1, \ldots, x_n\rangle \mid x_{\ell(j)} = h_j(x_1, \ldots, \hat{x}_{\ell(j)}, \ldots, x_n), \langle x_1, \ldots, \hat{x}_{\ell(j)}, \ldots, x_n\rangle \in V_j\}$$

where V_j is a measurable subset of $\mathbb{R}^{n-1}$, $c_1 < (\partial F/\partial x_{\ell(j)})(y) < c_2$ for all $y \in S_j$, and $c_1 > 0$, $c_2 < \infty$. Define

$$G_j(\lambda) = (2\pi)^{-n/2} \int_{S_j} e^{-i\lambda \cdot x} f(x)\, d\omega$$

For simplicity of notation we assume that $\ell(j) = n$. Then

$$G_j(\lambda) = (2\pi)^{-n/2} \int_{V_j} \exp(-i\lambda_n h_j(x_1, \ldots, x_{n-1}) - i \sum_1^{n-1} \lambda_i x_i) \times \left(\frac{f(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1}))}{\dfrac{\partial F}{\partial x_n}(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1}))} \right) dx_1 \cdots dx_{n-1}$$

so the same computation as in the proof of Theorem IX.38b implies that for $m < -\frac{1}{2}$, we can use the $(1 + \lambda^2)^m$ factor to control the λ_n integration and then the Plancherel theorem to conclude

$$\|G_j\|^2_{L^2_m(\mathbb{R}^n)} \leq C \int_{V_j} \frac{|f(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1})|^2}{\left| \dfrac{\partial F}{\partial x_n}(x_1, \ldots, x_{n-1}, h_j(x_1, \ldots, x_{n-1}) \right|^2} dx_1 \cdots dx_{n-1}$$

$$\leq \frac{C}{c_1} \|f\|^2_{L^2(M \cap S_j, d\omega)}$$

Summing from 1 to N we conclude that there is a constant $\tilde{C}$ so that $\|\mathscr{F}_M f\|_{L^2_m(\mathbb{R}^n)} \leq \tilde{C}\|f\|_{L^2(M, d\omega)}$ for all f. This proves (b).

We have just seen that $\mathscr{F}_M$: $L^2(M, d\omega) \to L^2_{-m}(\mathbb{R}^n)$ is bounded if $m > \frac{1}{2}$. We can identify $L^2_m(\mathbb{R}^n)$ with the dual of $L^2_{-m}(\mathbb{R}^n)$ by associating to each $f \in L^2_m(\mathbb{R}^n)$ the functional

$$g \mapsto \int_{\mathbb{R}^n} \overline{f(x)} g(x)\, dx$$

Thus, $\mathscr{F}^*_M$ maps $L^2_m(\mathbb{R}^n)$ boundedly into $L^2(M, d\omega)$. So we can uniquely associate with each $f \in W_m$ a function $T_M f = \mathscr{F}^*_M(\hat{f})$ in $L^2(M, d\omega)$, so that if $f \in \mathscr{S}(\mathbb{R}^n)$, this mapping is just the restriction of f to M. Moreover, $\|T_M f\|_{L^2(M, d\omega)} \leq \tilde{C}\|f\|_{W_m}$. ∎

One is often interested in knowing how the restriction maps change as the submanifold M changes. Consider the case where $M = S^{n-1}$, the $(n-1)$-sphere in $\mathbb{R}^n$, and let $S^{n-1}_\lambda = \{x \in \mathbb{R}^n \mid \sum_{i=1}^n x_i^2 - \lambda = 0\}$. Theorem IX.39 implies that the restriction map T_λ is a bounded map from $W_m(\mathbb{R}^n)$ into $L^2(S^{n-1}_\lambda, d\omega)$ for each λ if $m > \frac{1}{2}$. Define $(U_\lambda f)(x) = f(\lambda x)$; then U_λ: $L^2(S^{n-1}_\lambda, d\omega) \to L^2(S^{n-1}, d\omega)$. We would like to know the continuity properties of the family of maps $U_\lambda T_\lambda$: $W_m(\mathbb{R}^n) \to L^2(S^{n-1}, d\omega)$.

Definition A function g from a metric space $\langle X, \rho\rangle$ to a Banach space $\langle B, \|\cdot\|\rangle$ is called **Hölder continuous of order α**, $\alpha \in (0, 1]$, if for each $x \in X$, there is a $\delta > 0$ such that $\|g(x) - g(y)\| \leq C\rho(x, y)^\alpha$ for all y satisfying $\rho(x, y) < \delta$.

Theorem IX.40 Let $R_\lambda = U_\lambda T_\lambda$ be the family of restriction maps defined above with $m > \frac{1}{2}$. Then for each $f \in W_m(\mathbb{R}^n)$, $R_\lambda f$ is Hölder continuous of order α as an $L^2(S^{n-1}, d\omega)$-valued function of λ for each α with $0 < \alpha < m - \frac{1}{2}$.

Proof We sketch the proof leaving the details to the reader (Problem 58). Let $f \in L^2(S^{n-1}, d\omega)$ and define the dilated Fourier transform by

$$(\mathscr{F}^{(\lambda)} f)(k) = (2\pi)^{-n/2} \int_{S^{n-1}} e^{-ik \cdot \lambda x} f(x)\, d\omega$$

Notice that $|e^{-ik \cdot \lambda x} - e^{-ik \cdot \lambda' x}| \leq C|\lambda - \lambda'|^\alpha |k|^\alpha$ for any $\alpha \leq 1$. Using this, one proves that

$$\|\mathscr{F}^{(\lambda)} f - \mathscr{F}^{(\lambda')} f\|_{L^2_{-m}(\mathbb{R}^n)} \leq C|\lambda - \lambda'|^\alpha \|f\|_{L^2(S^{n-1}, d\omega)}$$

if $\alpha < m - \frac{1}{2}$. Since $R_\lambda f = (\mathscr{F}^{(\lambda)})^* \hat{f}$ (under the duality described in the proof of Theorem IX.39) we conclude from this that

$$\|R_\lambda f - R_{\lambda'} f\| \leq C_\alpha |\lambda - \lambda'|^\alpha \|f\|_{W_m}$$ ∎

We remark that it is possible to prove the following stronger result: Suppose $n + \frac{1}{2} < m \leq n + \frac{3}{2}$; then $R_\lambda f$, regarded as a map of $W_m(\mathbb{R}^n)$ into $L^2(S^{n-1}, d\omega)$ is n times differentiable and the nth derivative is Hölder continuous of order α for all $0 < \alpha < m - n - \frac{1}{2}$.

Our final topic in this section is the investigation of the map

$$f \mapsto \widehat{((k^2 - \lambda)^{-1} \hat{f})}$$

for λ positive. We are interested in this map because it is just the unbounded inverse $(-\Delta - \lambda)^{-1}$ for $\lambda > 0$. We will continue our study of $(-\Delta - \lambda)^{-1}$ in Section XIII.7, where we study the spectral properties of certain quantum-mechanical Hamiltonians. The idea of the following theorem is that $(k^2 - \lambda)^{-1}$ is singular only on $S^n_{\lambda^{1/2}}$, the sphere of radius $\lambda^{1/2}$, so if the restriction of $\hat{f}$ to $S^n_{\lambda^{1/2}}$ is zero we expect that $f \mapsto \widehat{(k^2 - \lambda)^{-1} \hat{f}}$ should not be too singular. For convenience, we denote the norm on $L^2_\alpha(\mathbb{R}^n)$ by $\|\cdot\|_\alpha$.

Theorem IX.41 Let $f \in L^2_\alpha(\mathbb{R}^n)$ for some $\alpha > \frac{1}{2}$ and suppose that the restriction of $\hat{f}$ (given by Theorem IX.39) to the sphere of radius $\lambda^{1/2}$ ($\lambda > 0$) is the zero function. Then for each $\varepsilon > 0$,

$$B_\lambda f \equiv \widehat{(k^2 - \lambda)^{-1} \hat{f}} \in L^2_{\alpha - 1 - 2\varepsilon}$$

Moreover, for each $\varepsilon > 0$, $\alpha > \frac{1}{2}$, and $\lambda > 0$, there is a constant C so that

$$\|B_\lambda f\|_{\alpha - 1 - 2\varepsilon} \leq C \|f\|_\alpha$$

for all $f \in L^2_\alpha(\mathbb{R}^n)$ such that $\hat{f}$ vanishes on $S^n_{\lambda^{1/2}}$. C remains bounded if λ varies through a compact subset of $(0, \infty)$.

We will prove Theorem X.41 by a series of lemmas. The first is a direct consequence of the fact that L^2_α is the set of Fourier transforms of the Sobolev space W_α and the proof of Proposition 2 in Section IX.6.

Lemma 1 Let F be a C^∞ function so that all the derivatives of F are bounded. Then $f \mapsto \widehat{(F\hat{f})}$ is a bounded map on each L^2_α.

Our technique for proving Theorem IX.41 will be to prove the theorem first in the case $n = 1$ and then to use this special case along with a "cutting and pasting" argument to do the general case.

Lemma 2 Let $f \in L^2_\alpha(\mathbb{R})$ with $\alpha > \frac{1}{2}$ (so that $f \in L^1(\mathbb{R})$). Suppose that $\int_{-\infty}^{\infty} f(x)\, dx = 0$. Then,

(a) There is a one-parameter family of tempered distributions satisfying $k\hat{g}(k) = \hat{f}(k)$. Each is a continuous function and there is a unique one g with $\lim_{x \to \pm\infty} g(x) = 0$.

(b) For each sufficiently small $\varepsilon > 0$, g obeys the bound

$$|g(x)| \leq C \|f\|_\alpha (1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \tag{IX.46}$$

where C depends only on α and ε.

Proof Let $g(x)$ be defined by

$$g(x) = i \int_{-\infty}^{x} f(y)\, dy = -i \int_{x}^{\infty} f(y)\, dy \tag{IX.47}$$

Suppose that $x < 0$ and choose $\varepsilon > 0$ small enough so that $\alpha > \frac{1}{2} + \varepsilon$. Then

$$|g(x)|^2 \leq \left| \int_{-\infty}^{x} |f(y)| (1 + |y|^2)^{\frac{1}{2}\alpha} (1 + |y|^2)^{-\frac{1}{4} - \frac{1}{2}\varepsilon} (1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)}\, dy \right|^2$$

$$\leq (1 + |x|^2)^{-(\alpha - \frac{1}{2} - \varepsilon)} \|f\|_\alpha^2 \int_{-\infty}^{\infty} (1 + |y|^2)^{-\frac{1}{2} - \varepsilon}\, dy$$

For $x \geq 0$, one uses a similar argument using the second equality in (IX.47). Since $f \in L^1(\mathbb{R})$, g is absolutely continuous and $g'(x) = if(x)$, thus $k\hat{g}(k) = \hat{f}(k)$. By the hypothesis on f, $g(x) \to 0$ as $x \to \pm\infty$. If g_β is another tempered distribution satisfying $k\hat{g}_\beta = \hat{f}$, then $k(\hat{g} - \hat{g}_\beta) = 0$, so $\hat{g} - \hat{g}_\beta$ has support at the origin. This implies that $\hat{g}_\beta - \hat{g}$ is a finite linear combination of the delta function and its derivatives. Since $k(\hat{g}_\beta - \hat{g}) = 0$, the coefficients of the derivative terms vanish, so $\hat{g}_\beta = \hat{g} + \beta\delta_0$. It follows that $g_\beta = g + \beta(2\pi)^{-1/2}$. This shows that $g_\beta \to 0$ at $\pm\infty$ if and only if $\beta = 0$. ∎

We can now prove the one-dimensional case of Theorem IX.41.

Lemma 3 Let $\lambda > 0$ and $\alpha > \frac{1}{2}$. Suppose that $h \in L^2_\alpha(\mathbb{R})$ and $\hat{h}(\pm\lambda^{1/2}) = 0$. Then, there is a continuous function g going to zero at ∞ so that $(k^2 - \lambda)\hat{g} = \hat{h}$. Moreover, g obeys

$$|g(x)| \leq D_\lambda \|h\|_\alpha (1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \tag{IX.48}$$

where D_λ is a constant depending only on λ, α, and ε. For fixed α and ε, D_λ is bounded for λ in any compact subset of $(0, \infty)$.

Proof By a simple argument using the formula $\widehat{e^{i\gamma x} f(x)} = \hat{f}(k - \gamma)$, one can see that Lemma 2 implies that if $\hat{h}(\gamma) = 0$, then there is a g obeying (IX.46) so that $(k - \gamma)\hat{g} = \hat{h}$. We will denote such a g by $\widehat{(k - \gamma)^{-1} \hat{h}}$. Choose

a C^∞ function χ so that $\chi(k) = 0$ if $k < -\frac{1}{2}\lambda^{1/2}$ and $\chi(k) = 1$ if $k > \frac{1}{2}\lambda^{1/2}$ and define

$$F_1(k) = (k + \lambda^{1/2})^{-1}\chi(k), \qquad F_2(k) = (k - \lambda^{1/2})^{-1}(1 - \chi(k))$$

so that $(k - \lambda^{1/2})^{-1}F_1 + (k + \lambda^{1/2})^{-1}F_2 = (k^2 - \lambda)^{-1}$. Let $f_i = \widetilde{F_i \hat{h}}$. By Lemma 1, $\|f_i\|_\alpha \le C_{i,\alpha}\|h\|_\alpha$. Let $\hat{g} = (k - \lambda^{1/2})^{-1}\hat{f}_1 + (k + \lambda^{1/2})^{-1}\hat{f}_2$. Then $(k^2 - \lambda)\hat{g} = \hat{h}$ and

$$\begin{aligned} |g(x)| &\le C[\|f_1\|_\alpha + \|f_2\|_\alpha](1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \\ &\le D\|h\|_\alpha(1 + |x|^2)^{-\frac{1}{2}(\alpha - \frac{1}{2} - \varepsilon)} \end{aligned}$$

That D_λ is bounded as λ runs through a compact subset of $(0, \infty)$ is a simple consequence of the above proof. ∎

Note that by (IX.48),

$$\int |g(x)|^2(1 + |x|^2)^{\alpha - 1 - 2\varepsilon}\, dx \le D^2\|h\|_\alpha^2 \int (1 + |x|^2)^{-\frac{1}{2} - \varepsilon}\, dx$$

so that Lemma 3 is, indeed, a strengthened version of Theorem IX.41 in the case $n = 1$.

Lemma 4 Let $f \in L^2_\alpha(\mathbb{R}^n)$ with $\alpha > \frac{1}{2}$ and suppose that $\hat{f}$ vanishes on the sphere of radius λ. Then for almost every $p \in \mathbb{R}^{n-1}$,

$$h_p(y) \equiv (2\pi)^{-(n-1)/2} \int e^{-i(p_1x_1 + \cdots + p_{n-1}x_{n-1})} f(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

is in $L^2_\alpha(\mathbb{R})$ and for almost every $p \in \mathbb{R}^{n-1}$ with $|p| \le \lambda$, $\hat{h}_p(\pm\sqrt{\lambda^2 - |p|^2}) = 0$.

Proof If f were in $L^1(\mathbb{R}^n)$, the conclusion of the lemma would be trivial, but we must work a little harder. Since $f(x_1, \ldots, x_{n-1}, y)(1 + \sum_1^{n-1} x_i^2 + y^2)^{\alpha/2}$ is in $L^2(\mathbb{R}^n)$, we know that $f(x_1, \ldots, x_{n-1}, y)(1 + y^2)^{\alpha/2}$ is in $L^2(\mathbb{R}^n)$. Thus, by the Plancherel theorem,

$$\int |h_p(y)|^2(1 + |y|^2)^\alpha\, dy\, d^{n-1}p < \infty$$

It follows that for almost all p, $h_p(\cdot) \in L^2_\alpha(\mathbb{R})$. Now, choose $f_m \in \mathscr{S}(\mathbb{R}^n)$ so that $\|f - f_m\|_\alpha \to 0$. By Theorem IX.39, $\hat{f}_m \to \hat{f}$ in $L^2(S_\lambda^{n-1})$. Therefore, by passing to a subsequence if necessary, we may assume that:

(1) $\hat{f}_m(p, \pm\sqrt{\lambda - |p|^2}) \to 0$ for almost all $p \in \mathbb{R}^{n-1}$ with $|p|^2 < \lambda$
(2) $\|f_m - f\|_\alpha \le 4^{-m}$.

Define

$$h_p^{(m)}(y) = (2\pi)^{-(n-1)/2} \int \exp\left(-i\sum_{i=1}^{n-1} p_i x_i\right) f_m(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

We claim that $\|h_p^{(m)} - h_p\|_{L^2_\alpha(\mathbb{R})} \to 0$ a.e. in p. For by the argument at the beginning of the proof $\int \|h_p^{(m)} - h_p\|_\alpha^2\, d^{n-1}p \le 4^{-2m}$. Thus, for each m, the set $U_m = \{p \mid \|h_p^{(m)} - h_p\|_\alpha < 2^{-m}\}$ has a complement with measure less than 4^{-m}. Let $T_m = \bigcap_{n \ge m} U_n$ and let μ denote Lebesgue measure. Then $\mu(\mathbb{R}^{n-1} \setminus T_m) \le 4^{-m+1}$ so $\mu(\mathbb{R}^{n-1} \setminus \bigcup_m T_m) = 0$. But on each T_m, $h_p^{(m)} \to h_p$ in $L^2_\alpha(\mathbb{R})$ so $\|h_p^{(m)} - h_p\|_\alpha \to 0$ for almost all p. Therefore, by Theorem IX.39, $\hat{h}_p^{(m)}(\pm\sqrt{\lambda^2 - |p|^2}) \to \hat{h}_p(\pm\sqrt{\lambda^2 - |p|^2}) = \hat{f}(p, \sqrt{\lambda^2 - |p|^2})$ for almost all p with $|p|^2 < \lambda$. Since $\hat{h}_p^{(m)}(\pm\sqrt{\lambda - |p|^2}) = \hat{f}_m(p, \pm\sqrt{\lambda - |p|^2})$, (1) implies that $\hat{h}_p(\pm\sqrt{\lambda - |p|^2}) = 0$. ∎

Lemma 5 Fix $\lambda > 0$ and let

$$V = \left\{k \,\middle|\, \sum_{i=1}^{n-1} |k_i|^2 + |k_n - \lambda^{1/2}|^2 < \tfrac{1}{4}\lambda\right\} \subset \mathbb{R}^n.$$

Let $f \in L^2_\alpha(\mathbb{R}^n)$, $\alpha > \frac{1}{2}$, and suppose that $\hat{f}$ has support in V and that $\hat{f}\,|S_\lambda^{n-1} = 0$. Then

$$B_\lambda f = \widetilde{(k^2 - \lambda)^{-1}\hat{f}} \in L^2_{\alpha - 1 - 2\varepsilon}(\mathbb{R}^n) \qquad \text{and} \qquad \|B_\lambda f\|_{\alpha - 1 - 2\varepsilon} \le C'\|f\|_\alpha.$$

Proof Define $h_p(y)$ as in Lemma 4 and notice that by the argument at the start of the proof of Lemma 4 we have

$$\int \|h_p\|_\alpha^2\, d^{n-1}p \le \|f\|_\alpha^2 \tag{IX.49}$$

By the hypotheses, $h_p = 0$ if $|p| > \frac{1}{2}\lambda^{1/2}$. For each p with $|p| < \frac{1}{2}\lambda^{1/2}$, we define $\hat{g}_p(k) = (k^2 - (\lambda - |p|^2))^{-1}\hat{h}_p(k)$. Then, by Lemma 3,

$$|g_p(y)|^2 \le D^2\|h_p\|_\alpha^2(1 + |y|^2)^{-(\alpha - 1/2 - \varepsilon)}$$

Since

$$g_p(y) = (2\pi)^{-(n-1)/2} \int \exp\left(-i\sum_{i=1}^{n-1} p_i x_i\right)(B_\lambda f)(x_1, \ldots, x_{n-1}, y)\, d^{n-1}x$$

the Plancherel theorem and (IX.49) imply that

$$\int |(B_\lambda f)(x_1, \ldots, x_n)|^2\, d^{n-1}x \le D^2\|f\|_\alpha^2(1 + |x_n|^2)^{-(\alpha - 1/2 - \varepsilon)}$$

There are now two cases to consider. If $\alpha - 1 - 2\varepsilon \leq 0$, then

$$(1 + |x|^2)^{\alpha - 1 - 2\varepsilon} \leq (1 + |x_n|^2)^{\alpha - 1 - 2\varepsilon}$$

so

$$\|B_\lambda f\|^2_{\alpha - 1 - 2\varepsilon} \leq \int |(B_\lambda f)(x_1, \ldots, x_n)|^2 (1 + |x_n|^2)^{\alpha - 1 - 2\varepsilon}\, d^n x$$

$$\leq D^2 \|f\|^2_\alpha \int (1 + |x_n|^2)^{-1/2 - \varepsilon}\, dx_n$$

On the other hand, if $\alpha - 1 - 2\varepsilon > 0$, we must use a subtler argument. Let $\mathbf{e}_n = (0, 0, \ldots, 1)$. If $\mathbf{e}$ is a unit vector sufficiently close to $\mathbf{e}_n$, then by mimicking the above argument one can show that

$$\int |(B_\lambda f)(x_1, \ldots, x_n)|^2 (1 + |\mathbf{x} \cdot \mathbf{e}|^2)^{\alpha - 1 - 2\varepsilon}\, d^n x \leq D_1^2 \|f\|^2_\alpha \quad \text{(IX.50)}$$

Choose unit vectors $\mathbf{v}_1, \ldots, \mathbf{v}_n$ near $\mathbf{e}_n$ so that $\{\mathbf{v}_i\}_{i=1}^n$ is a basis for $\mathbb{R}^n$. Then, there is a constant C so that

$$1 + |\mathbf{x}|^2 \leq C \sum_{i=1}^n (1 + |\mathbf{x} \cdot \mathbf{v}_i|^2)$$

Thus, for some other constant C'

$$(1 + |\mathbf{x}|^2)^{\alpha - 1 - 2\varepsilon} \leq C' \sum_{i=1}^n (1 + |\mathbf{x} \cdot \mathbf{v}_i|^2)^{\alpha - 1 - 2\varepsilon}$$

Therefore by (IX.50)

$$\|B_\lambda f\|^2_{\alpha - 1 - 2\varepsilon} \leq C' D_1^2 \|f\|^2_\alpha \quad \blacksquare$$

Proof of Theorem IX.41 By a simple compactness argument we can cover $\mathbb{R}^n$ by finitely many neighborhoods $V_1, \ldots, V_m$ so that

$$V_i = \{k \mid |k - \lambda^{1/2} e_i| < \tfrac{1}{2}\lambda^{1/2}\} \qquad \text{for} \quad i = 1, 2, \ldots, m - 2$$

where $e_1, \ldots, e_{m-2}$ are unit vectors and where

$$V_{m-1} = \{k \mid |k| \leq \tfrac{3}{4}\lambda^{1/2}\}, \qquad V_m = \{k \mid |k| \geq \tfrac{5}{4}\lambda^{1/2}\}$$

Choose C^∞ functions $\{\chi_i\}_{i=1}^m$, with $\operatorname{supp} \chi_i \subset V_i$, so that $\sum_{i=1}^m \chi_i = 1$. By Lemma 1, $\sum_{i=1}^m \|\widehat{\chi_i f}\|_\alpha \leq C_1 \|f\|_\alpha$. Therefore, by Lemma 1 for $i = m - 1$ and $i = m$ and Lemma 5 for $i \leq m - 2$,

$$\|B_\lambda f\|_{\alpha - 1 - 2\varepsilon} \leq \sum_{i=1}^m \|\widehat{(k^2 - \lambda)^{-1} \chi_i \hat{f}}\|_{\alpha - 1 - 2\varepsilon} \leq C_2 \|f\|_\alpha \quad \blacksquare$$

Strč prst skrs krk *A Czech tongue-twister*

IX.10 Products of distributions, wave front sets, and oscillatory integrals

In this section we wish to discuss some results connected with the problem of defining the product of two distributions. If $T \in \mathscr{S}'(\mathbb{R}^n)$ and $S \in \mathscr{O}_M^n$, then we have already defined ST (see Example 7 and Operation 1 in Section V.3). More singular products often occur in applications. For example, in the theory of the free quantum field, one would like to define $\theta(x - y)\Delta_+(x - y) + \theta(y - x)\Delta_+(y - x)$ where Δ_+ is the two-point function and

$$\theta(f) = \int_{x_0 \geq 0} f(x)\, d^4 x$$

The problem of defining products is not to define a single product TS but to define a product with reasonable properties for a large class of T and S. In the above example, both θ and Δ_+ are singular at $x = 0$, but in a sense which we will make precise, the singularities are compatible in a way which allows us to define $\theta\Delta_+$.

We will attack the problem of products in two steps. First, we will "localize" T and S in such a way that we need consider only the case where T and S are distributions of compact support. Secondly, we will use the fact that the Fourier transform of a product is the convolution of the Fourier transforms and try to define TS so that $\widehat{TS} = (2\pi)^{-n/2} \hat{T} * \hat{S}$. This way of looking at products will lead naturally to the notion of the wave front set of a distribution. We complete the section by developing a method for computing the wave front set of a class of distributions called oscillatory integrals. Finally we use this machinery to define the product discussed above.

We remark that we will not have occasion to use the elaborate techniques of oscillatory integrals again and that they can be avoided if one merely wants to define the product $\theta\Delta_+$. We have included these techniques partly as an introduction to a set of important ideas which have found application in partial differential equations. We mention some of these applications in the Notes.

As motivation and as an introduction to localization techniques we first consider the case where T and S are singular at different points in the following precise sense:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. We say that $x \in \mathbb{R}^n$ is a **regular point** of T if and only if there is a neighborhood U of x and a function F, which is C^∞ on U,

so that $T(f) = \int f(x)F(x)\,dx$ for all $f \in \mathscr{D}$ with $\operatorname{supp} f \subset U$. The complement of the regular points of T is called the **singular support** of T and will be denoted by $\operatorname{sing\,supp}(T)$.

From the definition, it is clear that:

Proposition The singular support of T is a closed subset of $\operatorname{supp} T$.

In one case, it is easy to define TS; we just localize the notion of product used in Section V.3.

Theorem IX.42 Let T and S be in $\mathscr{D}'(\mathbb{R}^n)$. Suppose that $\operatorname{sing\,supp}(T) \cap \operatorname{sing\,supp}(S) = \varnothing$. Then there is a unique $W \in \mathscr{D}'$ so that

(a) If $x \notin \operatorname{sing\,supp}(S)$ and $S = F$, a C^∞ function, near x, then $W = FT$ near x. That is, if $S(f) = \int F(x)f(x)\,dx$ for all f with $\operatorname{supp} f \subset U$, an open set about x, then $W(f) = T(Ff)$ for all f with $\operatorname{supp} f \subset U$.
(b) If $x \notin \operatorname{sing\,supp}(T)$ and $T = G$, a C^∞ function, near x, then $W = GS$ near x.

Proof Let us first prove that there is at most one such W. For suppose that W_1, W_2 satisfy (a), (b), and let f be given. Let B_R denote the ball of radius R. Since $\operatorname{sing\,supp}(T) \cap \operatorname{sing\,supp}(S) = \varnothing$, for any $x \in B_{2R}$, we can find a ball $B^{(x)}_{r(x)}$ of radius $r(x)$ about x so that $W_1(g) = W_2(g)$ for all g with $\operatorname{supp} g \subset B^{(x)}_{r(x)}$ since either (a) or (b) holds near x for both W_1 and W_2. Choose finitely many $x_1, \ldots, x_k$ in B_{2R} so that $\bigcup_{i=1}^k B^{(x_i)}_{r(x_i)/2} \supset \bar{B}_R$ and choose nonnegative $\chi_1, \ldots, \chi_k$ with

$$\chi_i \in C_0^\infty, \qquad \operatorname{supp} \chi_i \subset B^{(x_i)}_{r(x_i)}, \qquad \text{and} \qquad \chi_i \restriction B^{(x_i)}_{r(x_i)/2} \equiv 1$$

Define $h = \sum_{i=1}^k \chi_i$ and let χ be a C_0^∞ function identically one on B_R with support in N, a neighborhood of $\bar{B}_R$ on which h is bounded from below by a strictly positive constant. Then for every $f \in C_0^\infty$ with $\operatorname{supp} f \subset B_R$, we can write

$$f = f\sum_{i=1}^k \chi\chi_i h^{-1} = \sum_{i=1}^k f\chi_i h^{-1} \equiv \sum_{i=1}^k f_i$$

where $f_i = \chi_i h^{-1} f$ is C^∞ with $\operatorname{supp} f_i \subset B^{(x_i)}_{r(x_i)}$. By the above argument, $W_1(f_i) = W_2(f_i)$ so $W_1(f) = W_2(f)$. Since R was arbitrary, $W_1 = W_2$.

This proves uniqueness. Now suppose for each R we can construct a distribution W_R on $\mathscr{D}(B_R)$. Then, by the above uniqueness, the W_R must

agree on their common domain, i.e., if $R_2 > R_1$, then $W_{R_2} \restriction \mathscr{D}(B_{R_1}) = W_{R_1}$, so the W_R fit together to form a functional on $\mathscr{D}$ that is continuous since it is continuous on each $\mathscr{D}(B_R)$.

Now fix R. For each $x \in B_{2R}$, x is either a regular point for T or one for S, so pick $B^{(x)}_{r(x)}$ so that either $S \restriction B^{(x)}_{r(x)}$ is a C^∞ function F_x or $T \restriction B^{x}_{r(x)}$ is a C^∞ function G_x. As above, choose finitely many x_i and label them so that $x_1, \ldots, x_\ell$ have associated F's and $x_{\ell+1}, \ldots, x_k$ have associated G's. Also, as above, let $u_i = \chi\chi_i h^{-1}$ so that u_i is C^∞, $\operatorname{supp} u_i \subset B^{(x_i)}_{r(x_i)}$ and $\sum_{i=1}^k u_i = 1$ on $\bar{B}_R$. Define W_R by

$$W_R(f) = \sum_{i=1}^{\ell} T(F_{x_i} u_i f) + \sum_{i=\ell+1}^{k} S(G_{x_i} u_i f) \tag{IX.51}$$

That (IX.51) obeys (a) and (b) is left to the reader. ∎

The above procedure of defining $W(f)$ in terms of the functions $u_i f$ is known as localization. There is an important element in the above proof which implies that we do not lose anything by localization, i.e., that we can put the local pieces back together. This is the fact that the topology on $\mathscr{D}$ is defined locally, i.e., for a functional T on $\mathscr{D}$ to be continuous, we need only know that its restriction to each $\mathscr{D}(B_R)$ is continuous. This is not true of the topology on $\mathscr{S}$. In fact, one can take two tempered distributions T and S which have a product TS by Theorem IX.42 but the product is not a tempered distribution!

Example 1 Let F be the bounded C^∞ function $F(x) = \exp(ie^x)$. Since F is bounded, $F \in \mathscr{S}'$. Let F' be the distributional derivative of F. Certainly $F' \in \mathscr{S}'$. Applied to any $g \in \mathscr{D}$

$$F'(g) = \int g(x)(ie^x)F(x)\,dx \tag{IX.52}$$

although (IX.52) is not true for arbitrary $g \in \mathscr{S}$. Let $\bar{F}$ be the tempered distribution $\exp(-ie^x)$. As ordinary distributions, both $\bar{F}$ and F' have empty singular supports and so by Theorem IX.42 we can define an element W of $\mathscr{D}'$ with $W = -i\bar{F}F'$. In fact W is just e^x but e^x is not tempered (since any *positive* distribution which is tempered must be given by a polynomially bounded measure).

This example illustrates the unsuitability of localization techniques when dealing with tempered distributions. For example, F' is given locally by a C^∞ function, but it is not equal to any C^∞ function as an element of $\mathscr{S}'$.

Now we want to try to define products of distributions that may have some common singular support. The most important property of products which we want to preserve is their connection to convolutions via the Fourier transform. Of course, in general, elements $T \in \mathscr{D}'$ may not have a Fourier transform, but if we localize, i.e., consider some fT with $f \in \mathscr{D}$, then, by Theorem IX.12, $\widehat{fT}$ is an entire analytic function. Thus, we try:

Definition Let $T, S \in \mathscr{D}'$. We say that $W \in \mathscr{D}'$ is the **product** of T and S if and only if for each $x \in \mathbb{R}^n$, there exists some $f \in \mathscr{D}$, with $f = 1$ near x so that for each $k \in \mathbb{R}^n$:

$$\widehat{f^2 W}(k) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} \widehat{fT}(\ell)\widehat{fS}(k-\ell)\, d\ell \tag{IX.53}$$

where the integral in (IX.53) is absolutely convergent. If such a W exists, we say the **product of T and S exists.**

Theorem IX.43

(a) The product is well defined, i.e., there is at most one W satisfying the definition.
(b) If $f \in \mathscr{D}$ and $T \in \mathscr{D}'$, then fT exists and is given by the usual definition, i.e., $fT(g) = T(fg)$.
(c) If TS, $(TS)V$, SV, and $T(SV)$ all exist, then $T(SV) = (TS)V$; if TS exists, then ST exists and $TS = ST$.
(d) If T and S are distributions with disjoint singular supports, then TS exists and is given by the product W of Theorem IX.42.
(e) If T and S are distributions of compact support, a sufficient condition that TS exist is that $\int \hat{T}(\ell)\hat{S}(k-\ell)\, d\ell$ converge absolutely for each k and define a polynomially bounded function of k.
(f) A sufficient condition for $W = TS$ to exist is that for each $x \in \mathbb{R}^n$, there is some $f \in \mathscr{D}$ with $f(x) \neq 0$ so that the integral on the right-hand side of (IX.53) converges absolutely and yields a polynomially bounded function of k.
(g) If TS exists, then $\operatorname{supp}(TS) \subset \operatorname{supp} T \cap \operatorname{supp} S$.

Proof We will prove (a) and (g) and leave the rest to the problems. We first note that if (IX.53) holds, then for any $g \in \mathscr{D}$,

$$\widehat{gf^2 W} = (2\pi)^{-n/2}\widehat{gfT} * \widehat{fS} = (2\pi)^{-n/2}\widehat{fT} * \widehat{gfS} \tag{IX.54}$$

(IX.54) follows from the associativity $\hat{g} * (\widehat{fT} * \widehat{fS}) = (\hat{g} * \widehat{fT}) * \widehat{fS}$, which is true because the necessary change of variables is legitimate on account of the assumed absolute convergence of (IX.53). Thus, if W_1 and W_2 both satisfy the definition, then for each $x \in \mathbb{R}^n$ we can find f and g identically one near x so that $\widehat{f^2 W_1} = (2\pi)^{-n/2}\widehat{fT} * \widehat{fS}$ and $\widehat{g^2 W_2} = (2\pi)^{-n/2}\widehat{gT} * \widehat{gS}$. By (IX.54), we conclude that $\widehat{f^2 g^2 W_1} = \widehat{f^2 g^2 W_2}$, so $W_1 - W_2$ vanishes near x, and thus by the argument in Theorem IX.42, it is zero.

To prove (g) we need only show that if $x \notin \operatorname{supp} T$, then $x \notin \operatorname{supp}(TS)$ and evoke symmetry. By the argument in Theorem IX.42, it is sufficient to prove that $TS(f) = 0$ for all f with support in N, some small neighborhood of x. So choose N with $T(f) = 0$ if $\operatorname{supp} f \subset N$. Then $fT \equiv 0$ since for all $g \in \mathscr{D}$, $fT(g) = T(fg) = 0$. Thus, by (c), $f(TS) = (fT)S = 0$. Finally letting χ be any function in $\mathscr{D}$ identically one on N, we have $TS(f) = TS(f\chi) = (fTS)(\chi) = 0$. ∎

Example 2 Let $T = S = \delta$ in $\mathscr{D}(\mathbb{R})$. Then $\hat{T} = \hat{S} = (2\pi)^{-1/2}$ and for any f identically one near $x = 0$, $fT = T$ so that the integral (IX.53) diverges. Thus the product TS does not exist.

Example 3 $T = S = \mathscr{P}(1/x) - i\pi\delta(x)$ where $\mathscr{P}$ is the Cauchy principle value (Example 6 of Section V.3). As we have seen (Problem 22 of Chapter V),

$$T = \lim_{\varepsilon \downarrow 0} \frac{1}{x + i\varepsilon} \tag{IX.55}$$

Using (IX.55), it is easy to show (Problem 54) that

$$\hat{T}(k) = -(2\pi)^{-1/2}(2\pi i)\theta(k) \tag{IX.56}$$

where θ is the Heavyside function given in Example 8 of Section V.3. Thus

$$\begin{aligned}(2\pi)^{-1/2}\int \hat{T}(\ell)\hat{S}(k-\ell)\, d\ell &= -(2\pi)^{-3/2}(2\pi)^2 \int \theta(\ell)\theta(k-\ell)\, d\ell \\ &= -(2\pi)(2\pi)^{-1/2} k\theta(k) \\ &= (ik)\hat{T}(k)\end{aligned}$$

Thus, by (e) of the last theorem, TS exists and $TS = -T'$; explicitly,

$$(TS)(f) = \lim_{a \downarrow 0} \int_a^\infty \left(\frac{f(x) + f(-x) - 2f(0)}{x^2} \right) dx - i\pi f'(0)$$

Example 4 There is a simple generalization of Example 3 to distributions in $\mathbb{R}^n$. Namely, if T and S have Fourier transforms with supports in a convex cone with a dual cone C having nonempty interior, then it can be shown that $\hat{T} * \hat{S}$ exists. In this case there is an alternative way of defining TS (Problem 62); for since $\hat{T}$ has support in a cone, by Theorem IX.16 there is an analytic function $\tilde{T}$ on $\mathbb{R}^n + iC$ with $T = \lim_{\kappa \downarrow 0, \kappa \in C} \tilde{T}(\cdot + i\kappa)$. Then, since $\tilde{T}$ and $\tilde{S}$ are polynomially bounded as $\kappa \to 0$, so is $\tilde{T}\tilde{S}$ so that $\lim_{\kappa \downarrow 0; \kappa \in C} \tilde{T}(\cdot + i\kappa)\tilde{S}(\cdot + i\kappa)$ exists and defines a distribution. This is identical to the TS defined by our general procedure.

In Example 3, T and S are singular at $x = 0$, but their Fourier transforms are not badly behaved in all directions. This suggests that we single out singular directions as well as singular points:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. A point $\langle x, k\rangle \in \mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$ is called a **regular directed point** for T if and only if there is a neighborhood N of x, a neighborhood M of k, and a function $g \in \mathscr{D}$, identically one in N, so that for each $m > 0$, there is a constant C_m with

$$|S(\lambda p)| \equiv |\widehat{gT}(\lambda p)| \leq C_m(1 + |\lambda|)^{-m} \tag{IX.57}$$

for all $p \in M$, $\lambda \in \mathbb{R}_+ = [0, \infty)$. The complement in $\mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$ of the regular directed points for T is called the **wave front set** of T and denoted $WF(T)$.

Tlus $\langle x, k\rangle$ is a regular directed point if the localization gT of T near x has a Fourier transform falling off faster than any power in a cone about k (Figure IX.6).

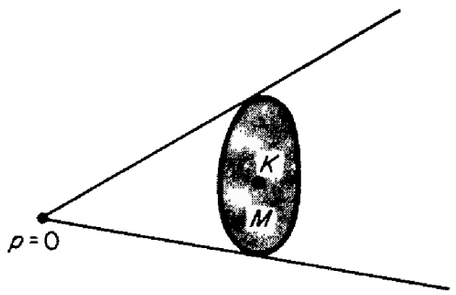


FIGURE IX.6 The cone $\bigcup_{\lambda>0}(\lambda M)$.

Theorem IX.44 Let $T \in \mathscr{D}'(\mathbb{R}^n)$. Then:

(a) $WF(T)$ is a closed subset of $\mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$.
(b) For each $x \in \mathbb{R}^n$,

$$WF_x(T) \equiv \{k \mid \langle x, k\rangle \in WF(T)\}$$

is a cone, i.e., $k \in WF_x(T)$ and $\lambda > 0$ implies $\lambda k \in WF_x(T)$.

(c) $WF(T + S) \subset WF(T) \cup WF(S)$.
(d) $\{x \mid WF_x(T) \neq \varnothing\}$ is sing supp(T).
(e) If $T \in \mathscr{S}'$ and $\hat{T}$ has support in a closed cone C, then for each x, $WF_x(T) \subset C$.
(f) Let M be a diffeomorphism of $\mathbb{R}^n$ to $\mathbb{R}^n$ (i.e., a C^∞ map with a C^∞ inverse) and let $T \circ M$ be the distribution

$$(T \circ M)(f) = T(g^{-1}(f \circ M^{-1}))$$

where g is the determinant of the Jacobian matrix dM_x given by $(dM_x)_{ij} = \partial M_i/\partial x_j$. Let $M_* : \mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\}) \to \mathbb{R}^n \times (\mathbb{R}^n\backslash\{0\})$ by

$$M_*\langle x, k\rangle = \langle M(x), dM_x^*(k)\rangle$$

where dM_x^* is the adjoint of dM_x with respect to the Euclidean inner product on $\mathbb{R}^n$. Then

$$WF(T \circ M) = M_*[WF(T)]$$

Proof (a)–(c) follow directly from the definition of $WF(T)$. For the case of linear coordinate change, (f) is easy, but in general a subtle argument is needed (Problem 75). To prove (d), we must show that x is a regular point if and only if $\langle x, k\rangle$ is a regular direction for all $k \in \mathbb{R}^n\backslash\{0\}$. The "only if" statement is clear, so suppose that $\langle x, k\rangle$ is a regular direction for each k. Then for each k in the unit sphere $S = \{k \mid |k| = 1\}$, there exist g_k, N_k, M_k so that (IX.57) holds. By the compactness of S, we can find $k_1, \ldots, k_m$ with $\bigcup_{i=1}^m M_{k_i} \supset S$. Let $g = \prod_i g_{k_i}$ and $N = \bigcap N_{k_i}$. By (IX.57) and the lemma below, $\widehat{gT}$ falls off faster than any power in each $\bigcup_{\lambda>0} \lambda\tilde{M}_{k_i}$, where $\tilde{M}_{k_i}$ is an arbitrary compact subset of M_{k_i}, and therefore in $\mathbb{R}^n\backslash\{0\}$. It follows that $\widehat{g^2T} = (2\pi)^{-n/2}\hat{g} * \widehat{gT}$ lies in $\mathscr{S}(\mathbb{R}^n)$ so that g^2T is C^∞. Since g is identically 1 near x, T is C^∞ near x.

To prove (e), choose f positive near x so that $\hat{f}$ has compact support. Then $\widehat{fT}(k) = \hat{T}(g_k)$ where $g_k(\ell) = (2\pi)^{-n/2}\hat{f}(\ell - k)$. If $k \notin C$, then for some small open set U about k, $\bar{U} \cap C = \varnothing$. For all large λ, supp $g_{\lambda\ell} \cap C = \varnothing$ for all $\ell \in U$ and so $\widehat{fT}(k)$ vanishes on λU for λ large. Now, given x, find $h \in \mathscr{D}$ so that hf is identically 1 near x. By the lemma, $\widehat{hfT}$ falls off faster than any power in $\bigcup_{\lambda>0} \lambda\tilde{U}$ where $\tilde{U}$ is a compact neighborhood of k in U. ∎

The following lemma completes the proof of Theorem IX.44.

Lemma Let M be an open set disjoint from 0 and suppose $S \in O_M^n$ obeys (IX.57) for $\lambda \in \mathbb{R}_+$, $k \in M$. Let $\tilde{M}$ be an arbitrary compact subset of M and let $h \in \mathscr{S}$. Then $h * S$ obeys (IX.57) for all $k \in \tilde{M}$, $\lambda \in \mathbb{R}_+$.

Proof Let $U = \bigcup_{\lambda>0} \lambda M$ and write

$$(S * h)\hat{}(\lambda k) = \int_{\ell \in U} S(\ell)h(\lambda k - \ell)\, d\ell + \int_{\ell \notin U} S(\ell)h(\lambda k - \ell)\, d\ell$$

On U, $|S(\ell)| \leq C_m(1 + |\ell|)^{-m}$ for any m and on all of $\mathbb{R}^n$, $|h(\ell)| \leq D_j(1 + |\ell|)^{-j}$ for all j. Now

$$|\lambda k| + 1 \leq |\lambda k - \ell| + |\ell| + 1 \leq (|\lambda k - \ell| + 1)(|\ell| + 1)$$

so that for any k,

$$\left| \int_{\ell \in U} S(\ell)h(\lambda k - \ell)\, d\ell \right| \leq \int D_j C_{j+n+1}(|\lambda k| + 1)^{-j}(|\ell| + 1)^{-n-1}\, d\ell$$
$$\leq (\text{const})(|\lambda k| + 1)^{-j}$$

Next let $\tilde{U} = \bigcup_{\lambda>0} \lambda \tilde{M}$ and let $\alpha = \sup\{\ell \cdot k \mid |\ell| = |k| = 1, \ell \notin U, k \in \tilde{U}\}$. Then by the compactness of $\tilde{M}$ and the openness of M, $\alpha < 1$. Thus for $\ell \notin U$, $k \in \tilde{U}$,

$$|\ell - k|^2 \geq |\ell|^2 + |k|^2 - 2\alpha|\ell||k| \geq (1 - \alpha)(|\ell|^2 + |k|^2)$$
$$\geq \tfrac{1}{2}(1 - \alpha)(|\ell| + |k|)^2$$

so $|\ell - k| \geq \beta(|\ell| + |k|)$ for suitable $\beta > 0$. Now, since $S \in O_M^n$, $|T(k)| \leq E(1 + |k|^p)$ for suitable p and $|h(\ell)| \leq D_{p+n+1+m}(1 + |\ell|)^{-(p+n+1+m)}$. Thus, for $k \in \tilde{U}$:

$$\left| \int_{\ell \notin U} S(\ell)h(\lambda k - \ell)\, d\ell \right| \leq ED_{p+n+1+m} \int (1 + |\lambda k| + |\ell|)^{-p-n-m-1}$$
$$\times (1 + |\ell|)^p\, d\ell \leq \text{const}(|\lambda k| + 1)^{-m}$$

Thus for $k \in \tilde{U}$,

$$|(S * h)(\lambda k)| \leq \text{const}(1 + |\lambda k|)^{-m}$$

Since $\inf\{|k| \mid k \in \tilde{M}\} > 0$, the lemma is proven. ∎

Example 2, revisited $WF(\delta) = \{\langle 0, \lambda\rangle \mid \lambda \neq 0\}$.

Example 3, revisited $WF(\mathscr{P}(1/x) - i\pi\delta(x)) = \{\langle 0, \lambda\rangle \mid \lambda > 0\}$.

If $\langle x, k\rangle \in WF(T)$, $\widehat{gT}$ is still polynomially bounded in direction k since gT is a tempered distribution. Thus, in "good" directions $\widehat{gT}$ falls off faster than any polynomial, while in "bad" directions it is polynomially bounded.

Thus, for any integral like $\int \widehat{gT}(\ell)\widehat{gS}(k - \ell)\, d\ell$ to converge, it is enough that each direction be good for either T or S. This suggests the following which is the first main theorem of this section:

Theorem IX.45 Let T and S be distributions. Suppose that

$$WF(T) \oplus WF(S) \equiv \{\langle x, k_1 + k_2\rangle \mid \langle x, k_1\rangle \in WF(T); \langle x, k_2\rangle \in WF(S)\}$$

does not contain any element of the form $\langle x, 0\rangle$. Then, the product TS exists and

$$WF(TS) \subset WF(T) \cup WF(S) \cup [WF(T) \oplus WF(S)] \qquad \text{(IX.58)}$$

Proof By definition, we need only define the product locally. So given $x \in \mathbb{R}^n$, let $\Gamma_1 = WF_x(T)$, $\Gamma_2 = WF_x(S)$. By hypothesis, $0 \notin \Gamma_1 + \Gamma_2$, so since Γ_1 and Γ_2 are closed, $\sup\{k_1 \cdot k_2 \mid k_1 \in \tilde{\Gamma}_1, -k_2 \in \tilde{\Gamma}_2\} < 1$ where we denote by $\tilde{C}$, $\{x \in C \mid |x| = 1\}$ for any cone C. For any closed cones K_1, K_2 in $\{\mathbb{R}^n \backslash 0\}$ with $\tilde{\Gamma}_1 \subset \tilde{K}_1^{\text{int}}$, $\tilde{\Gamma}_2 \subset \tilde{K}_2^{\text{int}}$, we can, by a compactness argument, find f identically one near x so that

$$|\widehat{fT}(k)| \leq c_j(1 + |k|)^{-j} \qquad \text{all } k \notin K_1, \text{ all } j \qquad \text{(IX.59)}$$

$$|\widehat{fS}(k)| \leq d_j(1 + |k|)^{-j} \qquad \text{all } k \notin K_2, \text{ all } j \qquad \text{(IX.60)}$$

Moreover, since fT and fS have compact support, there is an m and a D so that

$$|\widehat{fS}(k)| + |\widehat{fT}(k)| \leq D(1 + |k|)^m \qquad \text{all } k \qquad \text{(IX.61)}$$

Let us suppose that K_1, K_2 are chosen so "close" to Γ_1, Γ_2 that one has

$$\beta = \sup\{k_1 \cdot k_2 \mid k_1 \in \tilde{K}_1, -k_2 \in \tilde{K}_2\} < 1$$

Since the corresponding sup with K_i replaced by Γ_i is less than 1, this is always possible.

We will prove that the integral

$$I(k) = \int_{\ell_2 = k - \ell_1} \widehat{fS}(\ell_1)\widehat{fT}(\ell_2)\, d\ell_1$$

converges absolutely, is polynomially bounded, and falls off faster than any power in a neighborhood of any direction $k \notin K_1 \cup K_2 \cup (K_1 + K_2)$. This will prove the existence of the product by part (e) of Theorem IX.43 and

that $WF_x(TS) \subset K_1 \cup K_2 \cup (K_1 + K_2)$. Since K_i is an arbitrarily small cone about Γ_i, we will then have $WF_x(TS) \subset \Gamma_1 \cup \Gamma_2 \cup (\Gamma_1 + \Gamma_2)$ thereby concluding the proof of the theorem.

Decompose $I(k)$ as the sum of four integrals

$$I(k) = I_1(k) + I_2(k) + I_3(k) + I_4(k)$$

over the four regions $\ell_1 \in K_1, \ell_2 \in K_2$; $\ell_1 \in K_1, \ell_2 \notin K_2$; $\ell_1 \notin K_1, \ell_2 \in K_2$; $\ell_1 \notin K_1, \ell_2 \notin K_2$. We will often use the estimate of the lemma above that

$$|x| + 1 \leq (|y| + 1)(|x - y| + 1) \tag{IX.62}$$

By (IX.59), (IX.60) and (IX.62),

$$|I_4(k)| \leq c_j d_{n+j+1} \int (|\ell_1| + 1)^{-n-j-1}(|\ell_1 - k| + 1)^{-j}\, d\ell_1$$

$$\leq (|k| + 1)^{-j}\left[c_j d_{n+j+1} \int (|\ell_1| + 1)^{-n-1}\, d\ell_1\right]$$

so the integral in I_4 converges and falls off faster than any power in all directions.

Now $I_1(k) = 0$ unless $k \in K_1 + K_2$ so we need only prove the convergence of the integral and its polynomial boundedness to control the contribution of I_1, for it is automatic that $WF(I_1) \subset K_1 + K_2$. Now, if $\ell_1 \in K_1, \ell_2 \in K_2$, then

$$|\ell_1 + \ell_2|^2 \geq \tfrac{1}{2}(1 - \beta)(|\ell_1| + |\ell_2|)^2$$

Thus, for fixed k, the only ℓ's that enter in the integral I_1 have $|\ell_1|$, $|\ell_2| \leq 2(1 - \beta)^{-1}|k|$. Using (IX.61), we see that $I_1(k)$ converges and

$$I_1(k) \leq \int_{|\ell_1| \leq 2(1-\beta)^{-1}|k|} D^2[1 + 2(1 - \beta)^{-1}|k|]^{2m}\, d\ell_1$$

$$= D^2[1 + 2(1 - \beta)^{-1}|k|]^{2m+n} \times (\text{volume of unit ball})$$

Finally we consider I_2; the proof for I_3 is similar. By (IX.61) and (IX.60):

$$I_2(k) \leq D d_{j+m+n+1} \int_{k-\ell_2 \in K_1} (1 + |k - \ell_2|)^m (1 + |\ell_2|)^{-j-m-n-1}\, d\ell_2$$

If we ignore the $k - \ell_2 \in K_1$ condition and use $|k - \ell_2| \leq |k| + |\ell_2|$, we see that the integral converges and is polynomially bounded. We also claim that $I_2(k_0)$ falls off polynomially if $k_0 \notin K_1$, so that $WF(I_2) \subset K_1$. For if

$k_0 \notin K_1$, choose a cone K_3 about k_0 so that $\sup\{k_1 \cdot k_2 \,|\, k_1 \in \tilde{K}_1, k_2 \in \tilde{K}_3\} = \gamma < 1$. Then for $k \in K_3$, $k - \ell_2 \in K_1$, we have $|\ell_2| \geq \frac{1}{2}(1 - \gamma)(|k| + |k - \ell_2|)$, so that for $k \in K_3$,

$$I_2(k) \leq D d_{j+m+n+1} \int (1 + |\ell_1|)^m [1 + \tfrac{1}{2}(1 - \gamma)(|k| + |\ell_1|)]^{-j-m-n-1}\, d\ell_1$$

$$\leq \text{const}(1 + |k|)^{-j}$$

Thus $WF(I_2) \subset K_1$. By Theorem IX.44c,

$$WF(I) \subset \bigcup_{j=1}^{4} WF(I_j) \subset (K_1 + K_2) \cup K_1 \cup K_2. \blacksquare$$

Example 3, yet again $WF(\mathscr{P}(1/x) - i\pi\delta(x)) = \{\langle 0, \lambda\rangle \,|\, \lambda > 0\}$. Thus, by Theorem IX.45, all powers of $\mathscr{P}(1/x) - i\pi\delta(x)$ exist.

Example 5 Let x_1 and x_2 be the coordinates in $\mathbb{R}^2$ and let $\delta(x_1)$, $\delta(x_2)$ be defined in the usual way, e.g.

$$\int f(x_1, x_2)\delta(x_1)\, dx_1\, dx_2 = \int f(0, x_2)\, dx_2$$

Then

$$WF(\delta(x_1)) = \{\langle 0, x_2; \lambda, 0\rangle \,\big|\, x_2 \in \mathbb{R}, \lambda \neq 0\}$$

$$WF(\delta(x_2)) = \{\langle x_1, 0; 0, \lambda\rangle \,\big|\, x_1 \in \mathbb{R}, \lambda \neq 0\}$$

By the theorem, $\delta(x)\delta(y)$ exists and is clearly $\delta(x_1, x_2)$, the distribution taking f into $f(0)$.

To employ the machinery we have developed, one needs a method for computing wave front sets. We consider first a special example which we will then generalize sufficiently to compute the wave front set of the two-point function $\Delta_+(x; m^2)$ for a free quantum field.

Example 6 Let T_α be the Fourier transform of $(2\pi)^{-1/2}(1 + |k|^2)^\alpha$ in $\mathscr{S}'(\mathbb{R})$. If α is a positive integer n, then

$$T_n = \sum_{m=0}^{n} (-1)^m \binom{n}{m} \delta^{(2m)}(x)$$

clearly has support at zero with $WF(T_n) = \{\langle 0, \lambda\rangle \mid \lambda \neq 0\}$. One can also compute T_{-1} explicitly by a contour integration:

$$T_{-1}(x) = (2\pi)^{-1}\int_{-\infty}^{\infty} e^{-ikx}(1+k^2)^{-1}\,dk$$
$$= \tfrac{1}{2}e^{-|x|}$$

and more generally any T_{-n}. T_{-1} does not have $\{0\}$ as support, but it does have it as singular support. This suggests that, in general, T_α might have $\{0\}$ as singular support. How might we show this? If T_α is C^∞ away from zero, then we would expect $x^n T_\alpha$ to be *globally* smoother and smoother as n gets larger and larger. Moreover, if we can show for any m, there is an n with $x^n T_\alpha \in C^m(\mathbb{R})$, then clearly T_α is C^∞ away from zero. But

$$\widehat{x^n T_\alpha} = \left(i\frac{d}{dk}\right)^n \hat{T}_\alpha \equiv f_{\alpha,n}$$

where, by explicit computation

$$|f_{\alpha,n}(k)| \leq C(1+k^2)^{\alpha - n/2}$$

Thus, for any fixed α and m we can find n with $k^m f_{\alpha,n}(k) \in L^1$ (e.g. $n > m + 2\alpha + \frac{1}{2}$) and so T_α is C^∞ away from $x = 0$. Finally one can see that T_α is not smooth near zero. For by the Paley–Wiener idea and the fact that $(1+k^2)^\alpha$ is analytic in the strip $|\operatorname{Im} k| < 1$, T_α and its derivatives all fall off exponentially. If T_α were C^∞ at zero, T_α and thus $\hat{T}_\alpha$ would be in $\mathscr{S}$.

What was essential in the above argument was that all the derivatives of $\check{T}_\alpha$ fall off faster and faster, i.e., that it not behave like $x^{-n}\sin x$ whose derivatives are asymptotic to $\pm x^{-n}\sin x$ or $\pm x^{-n}\cos x$ at infinity. We thus define:

Definition *A* C^∞ function F on $\mathbb{R}^n$ is called a **symbol of order** k on $\{0\} \times \mathbb{R}^n$ if and only if for all $\alpha \in I_+^n$, there is a d_α with

$$|(D^\alpha F)(x)| \leq d_\alpha(1+|x|)^{(k-|\alpha|)}$$

A distribution F on $\mathbb{R}^n$ is called an **approximate symbol of order** k on $\{0\} \times \mathbb{R}^n$ if and only if, for any $\alpha \in I_+^n$, there exists a compact set S_α and a constant d_α so that F is equal to a $C^{|\alpha|}$ function outside S_α which satisfies

$$|(D^\alpha F)(x)| \leq d_\alpha(1+|x|)^{(k-|\alpha|)}$$

The phrase "on $\{0\} \times \mathbb{R}^n$" is included since this will be a special case of a definition to appear shortly. For the present, we suppress the phrase "on $\{0\} \times \mathbb{R}^n$."

Theorem IX.46 Let F be an approximate symbol of order k. Let $T = \hat{F}$. Then the singular support of T is either empty or $\{\langle 0, \ldots, 0\rangle\}$.

Proof The proof using the basic idea of Example 6 is left to the reader (Problem 66).

The above theorem does not cover many examples of interest: for example, we recall that $\Delta_+(x; m^2)$ has the form

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3}\int \exp(i\psi(x,k))\frac{d^3k}{\sqrt{m^2+k^2}}$$

with $\psi(x,k) = -x_0\sqrt{m^2+k^2} + \mathbf{x}\cdot\mathbf{k}$. This is something like the examples given in Theorem IX.46 but the phase factor is more complicated than $ik\cdot x$ and the integration variables are fewer than in the Fourier transform. We thus introduce a larger class of examples:

Definition Let Ω be an open set in $\mathbb{R}^n$. A function $a(\cdot,\cdot)\colon \Omega \times \mathbb{R}^s \to \mathbb{C}$ is called a **symbol of order** m on $\Omega \times \mathbb{R}^s$ if and only if, for each compact $K \subset \Omega$ and $\alpha \in I_+^n$, $\beta \in I_+^s$, there is a constant $d_{\alpha,\beta,K}$ with

$$|(D_x^\alpha D_\theta^\beta a)(x,\theta)| \leq d_{\alpha,\beta,K}(1+|\theta|)^{m-|\beta|} \tag{IX.63}$$

for all $x \in K$, $\theta \in \mathbb{R}^s$. The family of all symbols of order m with the seminorms

$$\|a\|_{\alpha,\beta,K} = \sup_{x\in K,\,\theta}(1+|\theta|)^{|\beta|-m}|(D_x^\alpha D_\theta^\beta a)(x,\theta)|$$

will be denoted by $\operatorname{Sym}(\Omega, s, m)$.

We say that $a(\cdot,\cdot)\colon \Omega \times \mathbb{R}^s \to \mathbb{C}$ is an **asymptotic symbol of order** m **on** $\Omega \times \mathbb{R}^s$ if and only if $a = a_1 + a_2$ with $a_1 \in \operatorname{Sym}(\Omega, s, m)$ and where (i) a_2 has compact support in the θ variables and (ii) the map $x \to a_2(x,\cdot)$ is C^∞ as a map from Ω to $L^\infty(\mathbb{R}^s)$.

Definition A **phase function** on $\Omega \times \mathbb{R}^s$ is a function $\varphi\colon \Omega \times \mathbb{R}^s \to \mathbb{R}$ such that

(i) φ is continuous and homogeneous of degree 1 in θ, i.e., $\varphi(x, \lambda\theta) = \lambda\varphi(x,\theta)$ for all $\langle x,\theta\rangle \in \Omega \times \mathbb{R}^s$ and $\lambda \geq 0$;

(ii) φ is C^∞ on $\Omega \times (\mathbb{R}^s \backslash \{0\})$;
(iii) φ has no critical points in $\Omega \times (\mathbb{R}^s \backslash \{0\})$, i.e., the $\mathbb{R}^n \times \mathbb{R}^s$-valued function $\langle \text{grad}_x \varphi, \text{grad}_\theta \varphi \rangle$ is never zero.

Definition An **oscillatory integral on** $\Omega \times \mathbb{R}^s$ is a formal expression

$$\int_{\theta \in \mathbb{R}^s} e^{i\varphi(x,\theta)} a(x, \theta)\, d\theta$$

where φ is a phase function and a is an asymptotic symbol.

Example 7 We can write

$$\Delta_+(x; m^2) = \frac{i}{2(2\pi)^3} \int e^{i\varphi(x,\theta)} a(x, \theta; m)\, d\theta$$

where

$$\varphi(x, \theta) = -x_0|\theta| + \mathbf{x} \cdot \theta$$
$$a(x, \theta; m) = (m^2 + |\theta|^2)^{-1/2} \exp(-ix_0[(m^2 + |\theta|^2)^{1/2} - |\theta|])$$

Let $\Omega = \mathbb{R}^4$. Clearly φ is a phase function since $\partial\varphi/\partial x_0 = |\theta| \neq 0$ if $\langle x, \theta \rangle \in \mathbb{R}^4 \times (\mathbb{R}^3 \backslash \{0\})$. The function a is not C^∞ because $|\theta|$ is not smooth at $\theta = 0$, but using $\left|\sqrt{m^2 + \theta^2} - |\theta|\right| \leq C(|\theta| + 1)^{-1}$, it is not hard to prove that a is an asymptotic symbol of order -1 (Problem 68). For example, let us show that $\partial a/\partial\theta_i$ falls off like $|\theta|^{-2}$ (for θ large). Let $f = (m^2 + \theta^2)^{-1/2}$ and $g = [(m^2 + |\theta|^2)^{1/2} - |\theta|.]$ Then

$$\left|\frac{\partial f}{\partial \theta_i}\right| = \left|\frac{\theta_i}{\theta}\right| \left|\frac{\theta}{(m^2 + \theta^2)^{-3/2}}\right| \leq c|\theta|^{-2} \qquad \text{for } \theta \text{ large}$$

and

$$\left|\frac{\partial g}{\partial \theta_i}\right| = \left|\frac{\theta_i}{\theta}\right| |[(m^2 + |\theta|^2)^{-1/2}\theta - 1]|$$
$$\leq [(1 + m^2|\theta|^{-2})^{-1/2} - 1] \leq c|\theta|^{-2}$$

Thus

$$\left|\frac{\partial a}{\partial \theta_i}\right| \leq \left|\frac{\partial f}{\partial \theta_i}\right| + \left|x_0 f \frac{\partial g}{\partial \theta_i}\right| \leq c|\theta|^{-2}$$

Since a is an asymptotic symbol, Δ_+ is an oscillatory integral.

We are heading toward a general theorem which will tell us that any oscillatory integral defines a distribution in a natural way and which identifies the wave front set of the distribution so defined. We first note two simple facts without proof (Problem 69):

Lemma 1 The C^∞ functions of compact support in $\Omega \times \mathbb{R}^s$ are dense in $\text{Sym}(\Omega, s, m)$ in the topology of $\text{Sym}(\Omega, s, m')$ whenever $m' > m$. In particular, a map from the functions of compact support to a topological space has at most one continuous extension to $\bigcup_{m<\infty} \text{Sym}(\Omega, s, m)$ continuous on each $\text{Sym}(\Omega, s, m)$ in its natural topology.

Lemma 2 Let $a(x, \theta)$ be a function of compact support in $\Omega \times \mathbb{R}^s$ so that $x \to a(x, \theta)$ is C^∞ as an L^∞-valued function on Ω. Then, for any phase function, $\int a(x, \theta) e^{i\varphi(x,\theta)}\, d\theta$ is a C^∞ function of x.

For the main theorem, we will need to define and develop one more concept:

Definition Let $\varphi(x, \theta)$ be a phase function on $\Omega \times \mathbb{R}^s$ where Ω is an open set in $\mathbb{R}^n$. Let

$$M(\varphi) = \{\langle x, \theta \rangle \in \Omega \times \mathbb{R}^s \backslash \{0\} \mid (\nabla_\theta \varphi)(x, \theta) = 0\}$$
$$SP(\varphi) = \{\langle x, (\nabla_x \varphi)(x, \theta) \rangle \mid \langle x, \theta \rangle \in M(\varphi)\} \subset \Omega \times \mathbb{R}^n$$

$SP(\varphi)$ is called **the manifold of stationary phase for** φ.

Lemma 3 $SP(\varphi)$ is a *closed* subset of $\Omega \times (\mathbb{R}^n \backslash \{0\})$ and if $\langle x, k \rangle \in SP(\varphi)$, then $\langle x, \lambda k \rangle \in SP(\varphi)$ for all $\lambda > 0$.

Proof Since φ is a phase function, it has no critical points so if $\langle x, \theta \rangle \in M(\varphi)$, then $\nabla_x \varphi \neq 0$. Thus $SP(\varphi) \subset \Omega \times (\mathbb{R}^n \backslash \{0\})$. If $\langle x, \theta \rangle \in SP(\varphi)$, then $\langle x, \lambda\theta \rangle \in SP(\varphi)$ since φ is homogeneous of degree one so that $(\nabla_x \varphi)(x, \lambda\theta) = \lambda(\nabla_x \varphi)(x, \theta)$. Finally, since $M(\varphi)$ is the set of zeros of a continuous function, it is closed. By a simple argument $\{x \mid M_x(\varphi) \neq \varnothing\}$ is closed. Since $\nabla_x \varphi$ is continuous, $SP(\varphi)$ is closed as the graph of a continuous function on a closed set. ∎

Example 7, continued $\varphi(x, \theta) = -x_0|\theta| + \mathbf{x} \cdot \theta$. Thus

$$\nabla_\theta \varphi = -x_0 \theta |\theta|^{-1} + \mathbf{x}$$

so

$$M(\varphi) = \{\langle x, \theta\rangle \mid x = 0\} \cup \{\langle x, \theta\rangle \mid |\mathbf{x}| = |x_0| \neq 0; \boldsymbol{\theta} = \lambda \mathbf{x}/x_0 \text{ with } \lambda > 0\}$$

Since $\nabla_x \varphi(x, \theta) = \langle -|\theta|, \boldsymbol{\theta}\rangle$ we conclude that

$$SP(\varphi) = \{\langle 0, 0; -|\theta|, \boldsymbol{\theta}\rangle | \boldsymbol{\theta} \in \mathbb{R}^3\}$$
$$\cup \{\langle \pm|\mathbf{x}|, \mathbf{x}; -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle | \mathbf{x} \in \mathbb{R}^3 \quad \text{and} \quad \lambda > 0\}$$

Thus $\{x \mid SP_x(\varphi) \neq \varnothing\}$ is the light cone $\{x \mid x_0 = \pm|\mathbf{x}|\}$, and $SP(\varphi)$ is the family of tangent vectors to the light cone which are lightlike and have negative time component (see Figure IX.7).

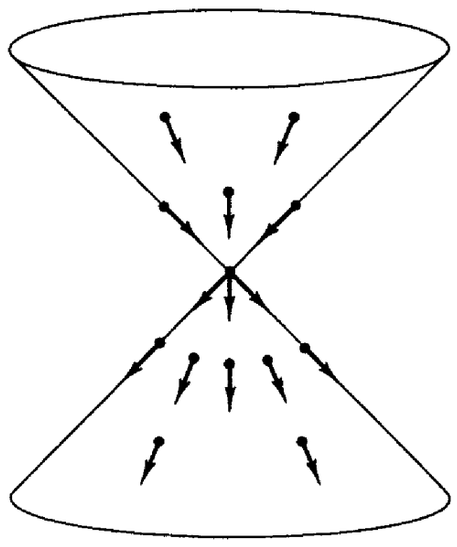


FIGURE IX.7 The set $SP(\varphi)$.

We come now to the second main theorem of this section.

Theorem IX.47 Let $\Omega \subset \mathbb{R}^n$ be a fixed open set and let $\varphi(x, \theta)$ be a fixed phase function on $\Omega \times \mathbb{R}^s$. Then, with each asymptotic symbol a on $\Omega \times \mathbb{R}^s$, we can associate a distribution $D_\varphi(a)$ on Ω so that:

(a) $a \to D_\varphi(a)$ is a linear map.
(b) If a has compact support in θ, then $D_\varphi(a)$ is the C^∞ function

$$\int_{\theta \in \mathbb{R}^s} a(x, \theta) e^{i\varphi(x, \theta)}\, d\theta$$

(c) The restriction of $D_\varphi(\cdot)$ to $\mathrm{Sym}(\Omega, s, m)$ is a continuous function from $\mathrm{Sym}(\Omega, s, m)$ to $\mathscr{D}'_\Omega$.

D_φ is uniquely determined by (a)–(c) and moreover:

(d) For any asymptotic symbol a, $WF(D_\varphi(a)) \subset SP(\varphi)$, the manifold of stationary phase for φ.

$D_\varphi(a)$ is denoted by the formal expression

$$D_\varphi(a) = \int a(x, \theta) e^{i\varphi(x, \theta)}\, d\theta$$

The main element of the proof is the development and exploitation of an "integration-by-parts" machine generalizing the fact $-ix^{-1}(d/dk)e^{ikx} = e^{ikx}$ used in analyzing Example 6:

Lemma 4 Let φ be a phase function on $\Omega \times \mathbb{R}^s$ with $\Omega \subset \mathbb{R}^n$. Then there exist functions $a_1, \ldots, a_s, b_1, \ldots, b_n$, and c on $\Omega \times \mathbb{R}^s$ so that

(1) $a_i \in \mathrm{Sym}(\Omega, s, 0)$; $i = 1, \ldots, s$
(2) $b_j \in \mathrm{Sym}(\Omega, s, -1)$; $j = 1, \ldots, n$
(3) $c \in \mathrm{Sym}(\Omega, s, -1)$
(4) ${}^tV e^{i\varphi} = e^{i\varphi}$

where V is the differential operator

$$V = \sum_{j=1}^{s} a_j \frac{\partial}{\partial \theta_j} + \sum_{k=1}^{n} b_k \frac{\partial}{\partial x_k} + c$$

and ${}^tV$ is its adjoint

$${}^tVf = -\sum_{j=1}^{s} \frac{\partial}{\partial \theta_j}(a_j f) - \sum_{k=1}^{n} \frac{\partial}{\partial x_k}(b_k f) + cf$$

Proof Since φ has no critical points on $\Omega \times (\mathbb{R}^s \backslash \{0\})$, the function $\eta(x, \theta)$ given by

$$\eta(x, \theta) = \sum_{k=1}^{n} \left(\frac{\partial \varphi}{\partial x_k}\right)^2 + |\theta|^2 \sum_{j=1}^{s} \left(\frac{\partial \varphi}{\partial \theta}\right)^2$$

is nonvanishing on $\Omega \times (\mathbb{R}^s \backslash \{0\})$. Moreover, since φ is homogeneous of order 1 in θ, η is homogeneous of order 2, i.e., $\eta(x, \lambda\theta) = \lambda^2 \eta(x, \theta)$. Let $\chi(\theta)$ be a function in $C_0^\infty(\mathbb{R}^s)$ identically one near $\theta = 0$ and let

$$\tilde{a}_j = -i(1 - \chi)\eta^{-1}|\theta|^2 \frac{\partial \varphi}{\partial \theta_j}$$

$$\tilde{b}_k = -i(1 - \chi)\eta^{-1} \frac{\partial \varphi}{\partial x_j}$$

$$\tilde{c} = \chi$$

Let $U = \sum_j \tilde{a}_j \partial/\partial\theta_j + \sum_k \tilde{b}_k \partial/\partial x_k + \tilde{c}$. Then $Ue^{i\varphi} = -i(1-\chi)\eta^{-1}(\eta i e^{i\varphi}) + \chi e^{i\varphi} = e^{i\varphi}$. Moreover $\tilde{a}_j, \tilde{b}_k$ are C^∞ functions which are homogeneous in θ near $\theta = \infty$ (e.g., $\tilde{a}_j(\lambda\theta, x) = \tilde{a}_j(\theta, x)$ if $\lambda > 1$, $\theta >$ radius of supp χ). As a result the derivatives of $\tilde{a}_j$ and $\tilde{b}_k$ are homogeneous near infinity in just the right way to guarantee that $\tilde{a}_j \in \mathrm{Sym}(\Omega, s, 0)$ and $\tilde{b}_k \in \mathrm{Sym}(\Omega, s, -1)$. Clearly $\tilde{c} \in \mathrm{Sym}(\Omega, s, -1)$. Letting $a_j = -\tilde{a}_j, b_j = -\tilde{b}_j, c = \tilde{c} - \sum_{j=1}^s \partial a_j/\partial\theta_j - \sum_{k=1}^n \partial b_k/\partial x_k$, the lemma is proven. ∎

Proof of Theorem IX.47 Let a be an asymptotic symbol and write $a = a_1 + a_2$ where a_1 has compact support and a_2 is a symbol. Then $D_\varphi(a_1)$ is determined by (b) and is C^∞ by Lemma 2. Moreover, if we can construct $D_\varphi(a_2)$ obeying (b) and (c), it is uniquely determined by Lemma 1.

We claim we are thus reduced to proving that $D_\varphi(a)$ defined by (b) extends continuously to $\bigcup_{m>0} \mathrm{Sym}(\Omega, s, m)$ (in the sense of (c)) and that for any symbol a, $WF(D_\varphi(a)) \subset SP(\varphi)$. For, if $WF(T) = \varnothing$, then $WF(T+S) \subset WF(S)$ and $WF(S) = WF(T+S-S) \subset W(T+S)$ so $WF(D_\varphi(a_1)) = \varnothing$ implies that $WF(D_\varphi(a)) = WF(D_\varphi(a_2)) \subset SP(\varphi)$.

Now, let a have compact support in $\Omega \times \mathbb{R}^s$ and be C^∞. Let $D_\varphi(a)$ be the distribution given by the C^∞ function $\int a(x,\theta)e^{i\varphi(x,\theta)}\,d\theta$. Fix $f \in \mathscr{D}_\Omega$. Then, for any integer p,

$$[D_\varphi(a)](f) = \int a(x,\theta)e^{i\varphi(x,\theta)}f(x)\,dx\,d\theta$$

$$= \int [({}^tV)^p e^{i\varphi(x,\theta)}]a(x,\theta)f(x)\,dx\,d\theta$$

$$= \int e^{i\varphi(x,\theta)}V^p(a(x,\theta)f(x))\,dx\,d\theta$$

so

$$|[D_\varphi(a)](f)| \le \int |V^p(a(x,\theta)f(x))|\,dx\,d\theta$$

Now, it is easy to see that $\langle a, f\rangle \mapsto af$ is a continuous bilinear map of $\mathrm{Sym}(\Omega, s, m) \times C_0^\infty(\Omega) \to \mathrm{Sym}(\Omega, s, m)$ and that V is a continuous map of $\mathrm{Sym}(\Omega, s, m)$ to $\mathrm{Sym}(\Omega, s, m-1)$ (Problems 70, 71). Thus $V^p(a(x,\theta)f(x))$ is a compactly supported symbol of order $m-p$ and, in particular,

$$|V^p(a(x,\theta)f(x))| \le |||a|||_p \|f\|_p (1+|\theta|)^{m-p}$$

for suitable norms $|||\cdot|||_p$ and $\|\cdot\|_p$ on $\mathrm{Sym}(\Omega, s, m)$ and $C_0^\infty(K)$ (support $f \subset K \subset \Omega$; K compact). Fixing $p > n+m$,

$$|D_\varphi(a)(f)| \le C_{p,K}|||a|||_p \|f\|_p$$

where $C_{p,K}$ is a constant only dependent on K and p. Thus the map $a \to D_\varphi(a)$ from $C_0^\infty(\Omega \times \mathbb{R}^s)$ to $\mathscr{D}'_\Omega$ extends to a continuous map from $\mathrm{Sym}(\Omega, s, m)$ to $\mathscr{D}'_\Omega$.

All that remains is to prove that $WF(D_\varphi(a)) \subset SP(\varphi)$ for any $a \in \mathrm{Sym}(\Omega, s, m)$. To do this, we must develop our machinery a little further:

Lemma 5 Let M be an open set in Ω and C a cone in $\mathbb{R}^n\backslash\{0\}$ so that $M \times C$ is disjoint from $SP(\varphi)$. Then there exist functions $A_1, \ldots, A_s$, $B_1, \ldots, B_n$ and D on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ so that:

(a) A_i, B_j, and D are C^∞ on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ and homogeneous of degree -1 *jointly* in $\langle k, \theta\rangle$, i.e., $A_i(x, \lambda k, \lambda\theta) = \lambda^{-1}A_i(x, k, \theta)$, etc.

(b) ${}^tV_k \exp(i\tilde{\varphi}) = \exp(i\tilde{\varphi})$ where

$$V_k = \sum_{j=1}^s A_j(x,k,\theta)|\theta|\frac{\partial}{\partial\theta_j} + \sum_{\ell=1}^n B_\ell(x,k,\theta)\frac{\partial}{\partial x_\ell} + D$$

and

$$\tilde{\varphi}(x,k,\theta) = \varphi(x,\theta) - k\cdot x$$

Proof Let

$$\tilde{\eta}(x,\theta,k) = |\theta|^2 \sum_{j=1}^s \left(\frac{\partial\varphi}{\partial\theta}\right)^2 + \sum_{\ell=1}^n \left(\frac{\partial\varphi}{\partial x_\ell} - k_\ell\right)^2$$

Then, by the definition of $SP(\varphi)$, $\tilde{\eta}$ is nonvanishing on $M \times [C \times (\mathbb{R}^s\backslash\{0\})]$. Define

$$A_j = +i\tilde{\eta}^{-1}|\theta|\frac{\partial\varphi}{\partial\theta_j}$$

$$B_\ell = +i\tilde{\eta}^{-1}\left(\frac{\partial\varphi}{\partial x_\ell} - k_\ell\right)$$

$$C = \sum_{j=1}^s \frac{\partial(|\theta|A_j)}{\partial\theta_j} + \sum_{k=1}^n \frac{\partial B_k}{\partial x_k}$$

Since $\tilde{\eta}$ is nonvanishing on $M \times C \times (\mathbb{R}^s\backslash\{0\})$ and homogeneous of degree 2 in $\langle k, \theta\rangle$ the lemma follows as in Lemma 3. ∎

Conclusion of the Proof of Theorem IX.47 Suppose $\langle x_0, k_0\rangle \notin SP(\varphi)$. Choose a neighborhood of $\langle x_0, k_0\rangle$, $M \times C$, as in Lemma 5. Let χ be a $C_0^\infty(\mathbb{R}^n)$ function with support in M identically one near x_0. For each

pair of positive integers m, n, we will find a continuous norm $|||\cdot|||_{(m,n)}$ on $\mathrm{Sym}(\Omega, s, m)$ so that

$$|\widehat{\chi D_\varphi(a)}(k)| \leq |||a|||_{(m,n)}(1 + |k|)^{-n} \qquad \text{for all } k \in C \tag{IX.64}$$

for any $a \in C_0^\infty(\Omega \times \mathbb{R}^s)$. By the continuity we have already proven, (IX.64) will extend to all $a \in \mathrm{Sym}(\Omega, s, m)$ thus proving that $\langle x_0, k_0\rangle \notin WF(D_\varphi(a))$. Choose $\psi(\theta)$ in $C_0^\infty(\mathbb{R}^s)$, identically one if $|\theta| < 1$ and identically zero if $|\theta| > 2$. Write $a = \psi a + (1 - \psi)a$. By Lemma 2, $\widehat{\chi D_\varphi(\psi a)}(k)$ obeys an estimate of the form (IX.64). For $k \in C$, write

$$\begin{aligned}
|\widehat{\chi D_\varphi((1-\psi)a)}(k)| &= \left|\int \exp(i\tilde{\varphi}(x,k,\theta))\chi(x)(1-\psi(\theta))a(x,\theta)\,dx\,d\theta\right| \\
&= \left|\int \exp(i\tilde{\varphi}(x,k,\theta))V_k^p[\chi(x)a(x,\theta)(1-\psi(\theta))]\,dx\,d\theta\right| \\
&\leq \int |V_k^p[\chi a(1-\psi)]|\,dx\,d\theta \qquad \text{(IX.65)}
\end{aligned}$$

We claim that $|V_k^p[\chi a(1-\psi)]| \leq |||a|||(|k| + |\theta|)^{-p}(1 + |\theta|)^m$, where $|||\cdot|||$ is a norm on $\mathrm{Sym}(\Omega, s, m)$, on account of the homogeneity properties of A, B, D in $\langle k, \theta\rangle$. Since $1 - \psi$ vanishes if $|\theta| < 1$, for all θ in the integral (IX.65), we can use

$$\begin{aligned}
(|k| + |\theta|)^{-1} &\leq (|k| + 1)^{-1} \\
(|k| + |\theta|)^{-1} &\leq (|\theta|)^{-1} \leq (\tfrac{1}{2} + \tfrac{1}{2}|\theta|)^{-1}
\end{aligned}$$

and so obtain (IX.64) by taking p sufficiently large and using the fact that the χ factor makes the x integration in (IX.65) finite. ∎

* * *

Throughout this chapter, we have developed various techniques for using the Fourier transform to analyze functions or distributions. Now, we can use these methods to analyze the distribution $\Delta_+(x, m^2)$.

Theorem IX.48 The two-point function $\Delta_+(x, m^2)$ of the free field has the following properties:

(a) Δ_+ is Lorentz invariant.
(b) $WF(\Delta_+) = \{\langle 0, 0; -|\theta|, \theta\rangle \mid \theta \in \mathbb{R}^3\}$
$\cup \{\langle \pm|\mathbf{x}|, \mathbf{x}, -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle \mid \mathbf{x} \in \mathbb{R}^3, \lambda > 0\}$

(c) There exist C^∞ functions f_s, f_t^+, and f_t^- on $(0, \infty)$ so that

$$\Delta_+(x; m^2) = \begin{cases} f_s(x^2; m^2) & \text{if } x^2 < 0 \\ f_t^+(x^2; m^2) & \text{if } x^2 > 0, x_0 > 0 \\ f_t^-(x^2; m^2) & \text{if } x^2 > 0, x_0 < 0 \end{cases}$$

where $x^2 = x \cdot \tilde{x} = x_0^2 - x_1^2 - x_2^2 - x_3^2$.
(d) For $y > 1, f_s(y^2) \leq C_\varepsilon \exp(-(m - \varepsilon)y)$.
(e) $\lim_{y\to\infty} |y|^{2n} f_t^\pm(y) = 0$.
(f) $f_t^+(y) = \overline{f_t^-(y)}$.

Proof (a) follows from the fact that Δ_+ is the Fourier transform of a Lorentz invariant measure. To prove (b) we note that, by our analysis of Example 7 and Theorem IX.47, $WF(\Delta_+)$ is contained in the set $S_0 \cup S_+ \cup S_-$ where $S_0 = \{\langle 0, 0, -|\boldsymbol{\theta}|, \boldsymbol{\theta}\rangle \mid \boldsymbol{\theta} \in \mathbb{R}^3\}$; $S_\pm = \{\langle \pm|\mathbf{x}|, \mathbf{x}, -\lambda|\mathbf{x}|, \mp\lambda\mathbf{x}\rangle \mid \mathbf{x} \in \mathbb{R}^3, \mathbf{x} \neq \mathbf{0}, \lambda > 0\}$. Moreover, since $\Delta_+$is Lorentz invariant, $WF(\Delta_+)$ must be Lorentz invariant which means that S_+ is either contained in $WF(\Delta_+)$ or disjoint from it. If S_+ were disjoint from $WF(\Delta_+)$, then Δ_+ would equal a C^∞ function on $\{\langle t, \mathbf{x}\rangle \mid t > 0\}$. Since we will see that $\Delta_+(t_0, \mathbf{x})$ and its derivatives fall off exponentially as $\mathbf{x} \to \infty$ with t_0 fixed, it would follow that for $t_0 > 0$ $\Delta_+(t_0, \cdot)$ was in $\mathcal{S}(\mathbb{R}^3)$. Since its Fourier transform is not even L^1, S_+ cannot be disjoint from $WF(\Delta_+)$. By (f), once we know that $S_+ \subset WF(\Delta_+)$, we can conclude that $S_- \subset WF(\Delta_+)$. Finally, since $WF(\Delta_+)$ is closed and $S_0 \subset \overline{S}_+$, we have $S_0 \subset WF(\Delta_+)$. (b) implies that the singular support of Δ_+ is $\{x \mid x^2 = 0\}$ so Δ_+ is C^∞ in the regions in question and Lorentz invariant. This proves (c).

To prove (d), consider the distribution on $\mathbb{R}^3$ whose Fourier transform is $(k^2 + m^2)^{-1/2}$. By the Paley–Wiener idea (Problem 76) and the fact that $(k^2 + m^2)^{-1/2}$ is analytic in a tube, this distribution falls off exponentially with any exponent $a < m - \varepsilon$. Since $\Delta_+(0, x)$ is this distribution (up to a constant) we have proven (d).

To prove (e), we note that formally

$$f_t^+(x^2; m^2) = \frac{i}{2(2\pi)^3}\int \exp(-i|x|\sqrt{m^2 + k^2})\,d^3k/\sqrt{k^2 + m^2}$$

By mimicking the analysis of Example 6, we see that $|x|^{2n} f_t^+(x^2; m^2)$ is bounded so long as $n \geq 2$ (Problem 72).

Finally, since $\hat{\Delta}_+$ is real, $\Delta_+(-x) = \overline{\Delta_+(x)}$ proving (f). ∎

Corollary The product $\theta(x_0)\,\Delta_+(x, m^2)$ exists where $\theta(x_0)$ is defined by $\theta(f) = \int_{x_0 \geq 0} f(x)\,d^3x$.

Proof $WF(\theta) = \{\langle 0, \mathbf{x}, \pm\lambda, 0\rangle \,|\, \mathbf{x} \in \mathbb{R}^3, \lambda \in \mathbb{R}_+\}$ so $WF(\theta) \oplus WF(\Delta_+)$ does not contain any vector of the form $\langle x, 0\rangle$. Thus, by Theorem IX.45, the product exists. ∎

NOTES

Section IX.1 J. Fourier's original argument for the inversion formula appears in his classic *La Théorie Analytique de Chaleur*, Didot, Paris, 1822. Although his argument would not be considered a "rigorous proof" by modern standards, it contained the main ideas of the proof we have presented. The approach of first defining the Fourier transform on $\mathscr{S}(\mathbb{R}^n)$ and $\mathscr{S}'(\mathbb{R}^n)$ and then restricting to the classical L^p spaces is due to L. Schwartz and is described in *Théorie des Distributions*, Vol. II, Hermann, Paris, 1954. Schwartz's lucid book is the basic reference for the study of the Fourier transform on spaces of distributions and the theory of convolutions of distributions.

The Hermite expansion discussed in the Appendix to Section V.3 can be used to provide short proofs of the Fourier inversion and Plancherel theorems since $\hat{\varphi}_n(k) = (-i)^n \varphi_n(k)$.

Section IX.2 The Riemann–Lebesgue lemma was first proven for a restricted class of functions in B. Riemann, "Ueber der Darstellbarkeit einer Function durch einen trigonometrische Reihe" in *Math. Werke*, Teubner, 1876, pp. 213–253, and for all of L^1 in H. Lebesgue, "Sur les Séries Trigonométriques," *Ann. Sci. Ecole Norm. Sup.* **20** (1903), 453–485. The Plancherel theorem appears in M. Plancherel, "Contribution à l'étude de la représentation d'un fonction arbitraire par des intégrales définies," *Rend. Circ. Mat. Palermo* **30** (1910), 289–335. The Hausdorff–Young theorem was first proven in W. Young: "Sur la généralisation du théorème de Parseval," *C. R. Acad. Sci. Paris Sér. A-B* **155** (1912), 30–33; and extended in F. Hausdorff, "Eine Ausdehnung des Parselvalschen Satzes über Fourierreihen," *Math. Z.* **16** (1923), 163–169.

The original proof of Bochner's theorem appears in S. Bochner, *Vorlesungen über Fouriersche Integrale*, Akademie-Verlag, Berlin, 1932. For a proof of the generalization to distributions, see Schwartz's book. The proof of Bochner's theorem which we give depends on Stone's theorem. Conversely, it is possible to derive Stone's theorem from Bochner's theorem, see E. Hopf: *Ergodentheorie*, Springer-Verlag, Berlin, 1937, or F. Riesz and B. Sz.-Nagy: *Functional Analysis*, Ungar, New York, 1955.

In some sense, the "natural" setting for the L^p theory of the Fourier transform is on an arbitrary locally compact abelian group; see Chapters XIV and XV.

Section IX.3 The close relationship between the support properties of a function and the analyticity properties of its Fourier transform was first developed by R. Paley and N. Wiener in *Fourier Transforms in the Complex Domain*, Amer. Math. Soc. Colloqium Publication, Providence, Rhode Island, 1934. Their work concerned L^2 functions and L^2 boundary values (see below). Nevertheless, a whole class of theorems relating support properties to analyticity properties are usually called Paley–Wiener theorems. The connection between analyticity and the Fourier Transform was further studied by E. C. Titchmarsh, *Introduction to the Theory of Fourier Integrals*, Oxford Univ. Press (Clarendon), London and New York, 1937. The generalization to distributions with compact support was first proven in L. Schwartz, "Transformation de Laplace des distributions," *Comm. Sém. Math. Lund*, tome suppl. dédié à M. Riesz (1952). A more detailed relation between support and analyticity for functions supported on compact, convex, balanced sets is given in Problem 22.

The idea of regarding the Fourier transforms of more general distributions as the boundary values of analytic functions is also due to Schwartz who proved that if $T \in \mathscr{S}'(\mathbb{R}^n)$ has support in a cone Γ, then $F(\lambda - i\eta t) = \widehat{e^{-i\eta \cdot x} T}$ has polynomial growth in the sense of estimates (i) and (ii) as $t \to \infty$ and as $t \to 0$. To prove this weaker version of one half of Theorem IX.16, one does not need the lemma of Bros–Epstein–Glaser. If $a \in \Gamma$, one chooses a C^∞ function φ so that supp $\varphi \in \Gamma - a$ and $\varphi(x) = 1$ for $x \in \overline{\Gamma}$. Then $F(\lambda - it\eta) = \widehat{e^{-i\eta \cdot x}\varphi(x)T}$ is analytic in $\mathbb{R}^n - i\Gamma^*$, satisfies the growth properties, and has $\hat{T}$ as a boundary value. However, to obtain the estimate (IX.13) which gives polynomial growth near the whole boundary of $\mathbb{R}^n - i\Gamma^*$, one needs the Bros–Epstein–Glaser lemma which was proven in J. Bros, H. Epstein, and V. Glaser, "On the connection between analyticity and Lorentz covariance of Wightman functions," *Comm. Math. Phys.* **6** (1967), 77–100. The proof we give of the second half of Theorem IX.16 is due to L. Gårding (unpublished). His proof is based on the ideas of Köthe and Tillman who realized that a necessary condition for an analytic function to have distribution boundary values on a smooth boundary is polynomial growth; see G. Köthe, "Die Randverteilungen Analytischer Funktionen," *Math. Z.* **57** (1952), 13–33 and H.-G. Tillman, "Randverteilungen analytischer Funktionen und Distributionen," *Math. Z.* **59** (1953), 61–83. We remark that we have stated and proved Theorem IX.16 for a spherically symmetric cone, $\Gamma_{a,\theta}$, but the same proof may be carried through for an arbitrary convex cone (Problem 23). Then Γ^* is given by $\Gamma^* = \{\eta \,|\, \eta \cdot x \geq 0 \text{ for all } x \in \Gamma\}$.

There is another formulation of the Paley–Wiener-type theorems in terms of L^2 functions. Suppose $f \in L^2(0, \infty)$. Then $F(\lambda - i\eta) = (2\pi)^{-1/2} \int_0^\infty e^{-i\lambda x} e^{-\eta x} f(x)\,dx$ satisfies

(i) F is an analytic function in the open lower half-plane,

(ii)
$$\sup_{\eta \geq 0} \left\{ \int_{-\infty}^{\infty} |F(\lambda - i\eta)|^2\,d\lambda \right\} < \infty$$

and

(iii)
$$\int_{-\infty}^{\infty} |F(\lambda - i\eta) - \hat{f}(\lambda)|^2\,d\lambda \to 0 \qquad \text{as} \quad \eta \to 0$$

by the Lebesgue dominated convergence theorem. That is, $F(\lambda - i\eta)$ takes on the boundary value $\hat{f}(\lambda)$ in the sense of L^2. Analytic functions in the open lower half-plane satisfying (i), (ii), and (iii) are said to belong to the **Hardy–Lebesgue class**, $\mathscr{H}^2(\mathbb{R})$. In the book by Paley and Wiener cited above, the converse statement is proven. Namely, if $F(\lambda - i\eta)$ is in the Hardy–Lebesgue class, then there is a function $f \in L^2(0, \infty)$ so that $F(\lambda - i\eta) = \widehat{e^{-\eta x} f}$ and $F(\lambda - i\eta) \xrightarrow{L^2} \hat{f}(\lambda)$ as $\eta \downarrow 0$. Another related theorem says that $\widehat{e^{-\eta x} f(x)} \in L^2(\mathbb{R})$ for all $\eta \in (\alpha, \beta)$, an open interval containing zero, if and only if $\hat{f}(\lambda)$ has an analytic continuation $\tilde{f}(\lambda - i\eta)$ to the strip $\alpha < \eta < \beta$ and $\int_{-\infty}^{\infty} |\tilde{f}(\lambda - i\eta)|^2\,d\lambda < \infty$ for each $\eta \in (\alpha, \beta)$. The reader can easily formulate the generalization of these theorems to several variables.

By Theorem IX.13, if a function f falls off faster than any exponential, then its Fourier transform is an entire function. There are connections between the type of the analytic function

and the detailed rate of falloff; see L. Ehrenpreis, *Fourier Analysis in Several Complex Variables*, Wiley (Interscience), New York, 1970.

Section IX.4 L^p estimates aroused interest very early in the development of functional analysis. Young's inequality was proven in W. Young, "The determination of the summability of a function," *Proc. London Math. Soc.* **12** (1913), 71–78. The Hardy–Littlewood inequality appeared in G. Hardy and J. Littlewood, "Some properties of fractional integrals, I" *Math. Z.* **27** (1928), 565–608. Earlier a similar inequality for sequence spaces appeared in G. Hardy, J. Littlewood, and G. Pólya, "The maximum of a certain bilinear form," *Proc. London Math. Soc.* **25** (1926), 265–268. Their work is essentially a generalization of Hilbert's work on the bilinear form $\sum_{m,n} a_n b_m/(n+m)$, see H. Weyl, *Singulare Integralgleichungen mit besonderer Beruchsichtigung des Fourierschen Integraltheorems*, Inaugural Dissertation, Göttingen, 1908. Sobolev proved his generalization by reducing to the case $n = 1$ in S. Sobolev, "Sur un théorème d'analyse fonctionelle," *Mat. Sb.* (Recueil Math.) **46** (1938), 471–496. The proof was greatly simplified in N. du Plessis, "Some theorems about the Riesz fractional integral," *Trans. Amer. Math. Soc.* **80** (1955), 124–134.

The Hausdorff–Young theorem states: if $p^{-1} + q^{-1} = 1$ and $1 \le p \le 2$, then the norm of the Fourier transform from L^p to L^q is less than or equal to $(2\pi)^{n(1/2-1/p)}$. It has recently been proven in W. Beckner, "Sharp inequalities in Fourier Analysis," *Bull. Amer. Math. Soc.* (to appear) that the norm is actually equal to

$$C(p, q) = \left[\left(\frac{p}{2\pi}\right)^{1/p} \Big/ \left(\frac{q}{2\pi}\right)^{1/q}\right]^{1/2}$$

That the norm could not be smaller than this constant can be seen from the fact that $\|\hat{f}\|_q = C(p, q)\|f\|_p$ if $f = e^{-x^2/2}$.

The Riesz–Thorin theorem was first proven by M. Riesz, "Sur les maxima des formes bilinéaires et sur les fonctionelles linéaires," *Acta Math.* **49** (1926), 465–497. The idea of using complex methods to prove the theorem is due to C. Thorin, "Convexity Theorems," *Comm. Sém. Math. Lund*, **9** (1948). The idea of extending the Riesz–Thorin theorem to analytic families is due to E. Stein, "Interpolation of Linear Operators," *Trans. Amer. Math. Soc.* **83** (1956), 482–492.

Before the weak L^p spaces were formally defined, inequalities were proven which we would now describe as saying that a certain map is bounded from L^p to weak L^p. The weak L^p spaces were then a natural abstraction. The inequalities appeared first in the L^1 context in G. Hardy and J. Littlewood, "A maximal theorem with function theoretic applications," *Acta Math.* **54** (1930), 81–116, and then in the L^p context in the Marcinkiewicz paper quoted below.

The Marcinkiewicz theorem was announced in J. Marcinkiewicz, "Sur l'interpolation d'operateurs," *C. R. Acad. Sci. Paris* **208** (1939), 1272–1273, and was proven in full generality by A. Zygmund, "On a theorem of Marcinkiewicz concerning interpolation of operators," *J. Math.* **35** (1956), 223–248. Hunt's theorem appeared in R. Hunt, "An extension of the Marcinkiewicz theorem to $L(p, q)$ spaces," *Bull. Amer. Math. Soc.* **70** (1964), 803–807.

The $L(p, q)$ spaces are a generalization of the weak L^p spaces and were introduced by G. Lorentz in "On some new functional spaces," *Ann. Math.* **51** (1950), 37–55. Suppose that $\langle M, \mu\rangle$ is a measure space. For each measurable function f on M we can define a measurable function on $\mathbb{R}$ by

$$f^*(x) = \inf\{y > 0 \mid \lambda_f(y) \le x\}$$

where $\lambda_f(y) = \mu\{x \mid |f(x)| > y\}$ is the distribution function of f. Now define $L(p, q)$ to be the set of functions on M so that $\|f\|^*_{p,q} < \infty$ where

$$\|f\|^*_{pq} = \begin{cases} \left(\frac{q}{p}\int_0^\infty [t^{1/p} f^*(t)]^q \frac{dt}{t}\right)^{1/q}, & 1 < p < \infty \\ & 1 < q < \infty \\ \sup_{t>0}\{t^{1/p} f^*(t)\}, & 1 < p \le \infty, q = \infty \end{cases}$$

Thus $L^p = L(p, p)$ and $L^p_w = L(p, \infty)$. In fact, it can be shown that if $1 < q_1 \le p \le q_2 \le \infty$, then

$$L(p, q_1) \subset L^p \subset L(p, q_2) \subset L^p_w$$

For a discussion of these spaces and the related interpolation theorems see R. Hunt, "On $L(p, q)$ spaces," *Enseignement Math.* **12** (1966), 247–276. A very readable discussion of interpolation theorems (in particular, a proof of the Marcinkiewicz theorem) may be found in E. Stein and G. Weiss: *Introduction to Fourier Analysis on Euclidean Spaces*, Princeton Univ. Press, Princeton, New Jersey, 1971.

The abstract interpolation theory which we present in the appendix to Section IX.4 is due to A. Calderón, "Intermediate spaces and interpolation, the complex method," *Studia Math.* **24** (1964), 113–190 and J. Lions, "Théorèmes de traces et d'interpolation I, II," *Ann. Scuola Norm. Sup. Pisa* **13** (1959), 389–403; **15** (1960), 317–331; III: *J. Math. Pures Appl.* **42** (1963), 195–203. There are other methods of abstract interpolation. For a description of these and related topics, see the review article by S. Krein and I. Petunin, "Scales of Banach spaces," *Russian Math. Surveys* **21** (1966), 83–157.

The Hadamard three line theorem is just one of a large class of theorems called Phragmén–Lindelöf theorems which are essentially generalizations of the maximum principle to certain unbounded domains. The original papers are E. Phragmén, "Sur une extension d'un théorème classique de la théorie des fonctions," *Acta Math.* **28** (1904), 351–368 and E. Lindelöf and E. Phragmén, "Sur une extension d'un principe classique de l'analyse et sur quelques propriétés des fonctions monogènes dans le voisinage d'un point singulièr," *Acta Math.* **31** (1908), 381–406. In the bounded case, the three line theorem was announced in J. Hadamard, "Sur les fonctions entières," *Bull. Soc. Math. France* **24** (1896), 186–187.

The material discussed in Example 2 of the Appendix is a special case of noncommutative integration theory. In general one would like to define analogues of the L^p spaces for any von Neumann algebra (in our case the algebra is just $\mathscr{L}(\mathscr{H})$). The basic references for this theory are J. Dixmier, "Formes linéaires sur un anneau d'opérateurs," *Bull. Soc. Math. France* **81** (1953), 9–39; I. Segal, "A non-commutative extension of abstract integration," *Ann. Math.* **57** (1953), 401–457, *Correction* **58** (1953), 595–596: and R. Kunze, "$\mathscr{L}_p$ Fourier transforms on locally compact unimodular groups," *Trans. Amer. Math. Soc.* **89** (1958), 519–540. Some of the proofs we use follow the ideas and suggestions of E. Nelson, "Notes on non-commutative integration," *J. Functional Analysis* **15** (1974), 103–116.

Section IX.5 The Malgrange–Ehrenpreis theorem was proven independently by B. Malgrange: "Existence et approximation des solutions des équations aux dérivées partielles et des equations de convolution," *Ann. Inst. Fourier (Grenoble)* **6** (1955–56), 271–355, and L. Ehrenpreis: "Solution of some problems of division," *Amer. J. Math.* **76** (1954), 883–903. The use of fundamental solutions has long been a standard technique in the theory of ordinary differential equations and elliptic boundary-value problems. For an introduction to these methods, see R. Courant and D. Hilbert, *Methods of Mathematical Physics*, Vol. I, p. 351.

Wiley (Interscience), 1953. For a more advanced approach, the reader should consult the four books by Stakgold, Friedmann, Agmon, and Hörmander referred to in the Notes to Section V.4.

The Malgrange-Ehrenpreis theorem shows that the equation $P(D)f = \delta$ has a solution in $\mathscr{D}'(\mathbb{R}^n)$. It is a natural question to ask whether there is a solution that lies in $\mathscr{S}'(\mathbb{R}^n)$. This question was answered in the affirmative by L. Hörmander who proved the stronger statement that $P(D)[\mathscr{S}'] = \mathscr{S}'$ in "On the division of generalized functions by polynomials," *Ark. Mat.* **3** (1958), 555–568. For a general discussion of the ranges of constant coefficient partial differential operators on various spaces of distributions, see M. Agranovich, "Partial differential equations with constant coefficients," *Russian Math. Surveys* **16** (1961), 23–91.

Section IX.6 Weyl's lemma is due to H. Weyl: "The method of orthogonal projection in potential theory," *Duke Math. J.* **1** (1940), 414–444. Sobolev's lemma and spaces were introduced in S. L. Sobolev: "Sur un théorème d'analyse fonctionelle," *Mat. Sb.* **45** (1938), 471–496 and *Certaines applications de l'analyse fonctionelle à la physique mathématique*, Leningrad, 1945.

Weyl's lemma has many generalizations; we will describe two of them. Let Ω be an open bounded set in $\mathbb{R}^n$ and let $C_{\alpha\beta}(x)$, $0 \le |\alpha|, |\beta| \le m$, be a collection of m times continuously differentiable functions. The differentiable operator $A = \sum_{|\alpha|, |\beta| \le m} (-1)^{|\alpha|} D^\alpha C_{\alpha\beta}(x) D^\beta$ is said to be **strongly elliptic** if

$$\operatorname{Re}\left\{ \sum_{|\alpha|, |\beta| = m} C_{\alpha\beta}(x)\xi^\alpha \xi^\beta \right\} \ge C_0 |\xi|^{2m}, \qquad C_0 > 0$$

for all $x \in \Omega$ and all real vectors $\xi \in \mathbb{R}^n$. The following theorem is due to K. O. Friedrichs: "Differentiability of solutions of elliptic partial differential equations," *Math. Scand.* **1** (1953), 55–72.

Theorem Let φ be a weak solution of $A\varphi = f$. If $f \in W_k(\Omega)$, then $\varphi \in W_{k+2m}(\Omega)$.

In "On the theory of general partial differential operators," *Acta Math.* **94** (1955), 161–248, L. Hörmander introduced the following definition. A constant coefficient operator $P(D) = P(i^{-1}\partial/\partial x_1, \ldots, i^{-1}\partial/\partial x_n)$ on Ω (open, not necessarily bounded) is said to be **hypoelliptic** if whenever $f \in C^\infty(\Omega)$, every distribution solution φ of $P(D)\varphi = f$ which is locally L^2 in Ω is in $C^\infty(\Omega)$. Hörmander then proved:

Theorem $P(D)$ is hypoelliptic if and only if for every large constant M_1 there is a positive M_2 so that every zero $\zeta = \xi + i\eta$ of $P(\zeta)$ which satisfies $|\eta| \le M_2$ also satisfies $|\zeta| \le M_1$.

The reader can easily check that Δ is hypoelliptic but $\partial^2/\partial x^2 - \partial^2/\partial t^2$ is not. This theorem has various generalizations to nonconstant coefficient operators, see: L. Hörmander, "On the interior regularity of the solutions of partial differential equations," *Comm. Pure Appl. Math.* **9** (1958), 197–218; B. Malgrange, "Sur une classe d'opérateurs différentielles hypoelliptiques," *Bull. Soc. Math. France* **85** (1957), 283–306; and J. Peetre, "A proof of the hypoellipticity of formally hypoelliptic differential operators," *Comm. Pure Appl. Math.* **16** (1961), 737–747.

Sobolev's lemma (and thus the resulting regularity theorems) can be generalized to various L^p spaces. We say that a function f is in $L^p_k(\mathbb{R}^n)$ if all the partial derivatives of order less than or equal to k are in $L^p(\mathbb{R}^n)$. The generalization of Sobolev's lemma states:

Theorem Suppose that k is a positive integer and $q^{-1} = p^{-1} - k/n$.

(a) If $q < \infty$ (i.e., $p < n/k$), then $L^p_k(\mathbb{R}^n) \subset L^q(\mathbb{R}^n)$ and the natural inclusion map is continuous.

(b) If $q = \infty$ (i.e., $p = n/k$), then the restriction of any $f \in L^p(\mathbb{R}^n)$ to a compact subset of $\mathbb{R}^n$ belongs to $L^r(\mathbb{R}^n)$ for every $r < \infty$.

(c) If $p > n/k$, then every $f \in L^p_k(\mathbb{R}^n)$ can be modified on a set of measure zero so that the resulting function is continuous.

A proof of this theorem and related results may be found in E. Stein, *Singular Integrals and Differentiability Properties of Functions*, Princeton Univ. Press, Princeton, New Jersey, 1970.

The Sobolev inequalities which we have discussed bound an L^q-norm of a function by its L^p-norm and the L^p-norms of some of its derivatives. In some special cases, one can bound the L^q-norm of a function just by the L^p-norms of derivatives if the function is small near infinity. For example, in Section X.13 we will prove and use the estimate

$$\|f\|_6 \le C \sum_{i=1}^{3} \left\| \frac{\partial f}{\partial x_i} \right\|_2$$

for functions on $\mathbb{R}^3$.

Section IX.7 Most of this section is standard folk wisdom. Theorem IX.31 is due to J. Dollard, "Asymptotic Convergence and the Coulomb Interaction," *J. Math. Phys.* **5** (1964) 729–738.

Section IX.8 The Gårding-Wightman axioms were formulated by L. Gårding and A. S. Wightman in the early 1950's, but they felt it would be premature to publish them until nontrivial examples existed. However, preliminary versions of the axioms appeared in various places, and on the basis of these axioms, the Haag-Ruelle scattering theory was developed (see Section XII.15). This was, in turn, such a beautiful and physical theory that it motivated the publication of the axioms in A. S. Wightman and L. Gårding, "Fields as operator-valued distributions," *Ark. Fys.* **28** (1964), 129–189.

The axioms are thoroughly discussed and many consequences are derived in the two books: *PCT, Spin and Statistics, and All That*, Benjamin, New York, 1964, by R. F. Streater and A. S. Wightman; *The General Theory of Quantized Fields*, Amer. Math. Soc., Providence, Rhode Island, 1965, by R. Jost. These books also contain many references to early work in the subject.

The first question that naturally arises about the Wightman axioms is whether they are consistent. This is not a trivial question since so many mathematical structures are involved. In fact, if the commutator in the local commutativity axiom is changed to an anticommutator, then the axioms are inconsistent (see the spin-statistics theorem below). In Section X.7 we show that the axioms are consistent by showing that, for each m, they are satisfied by the free Klein-Gordon field of mass m. It has not been proven that there are any really interesting field theory models in four space-time dimensions involving interacting particles that satisfy the Wightman axioms. Recently, models obeying the analog of the Wightman axioms in two dimensions have been constructed: see, for example, *Constructive Quantum Field Theory* (G. Velo and A. S. Wightman, eds.), Springer-Verlag, Berlin, 1973, and references therein or B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton University Press, 1974.

Since we still do not possess large classes of mathematical models, let alone a theory, to describe completely the phenomena of elementary particle physics, there has been a great deal of "experimentation" with axioms. This experimentation has consisted of slightly changing the axioms, finding equivalent axiom schemes, or formulating axiom schemes based on some fundamental structures other than the local field structure of the Gårding-Wightman axioms.

If we wish to perturb the axioms slightly, one candidate for change is the purely technical axiom that specifies the test function space be $\mathscr{S}(\mathbb{R}^4)$. In fact, there is a folk theorem that

assures as that a class of formal models known as nonrenormalizable Lagrangian models will lead to Wightman functions which are not polynomially bounded in the tube. This can only be true if a test function space other than $\mathscr{S}(\mathbb{R}^4)$ is used. A whole class of alternative test function spaces which still allow one to phrase the microscopic causality condition are proposed and developed in A. Jaffe, "High energy behavior in quantum field theory, strictly localizable fields," *Phys. Rev.* **158** (1967), 1454–1461.

There are two types of equivalent reformulations of the Wightman axioms. The first is due to Wightman, who wrote down a set of postulates for a sequence of tempered distributions $\{\mathscr{W}_n | \mathscr{W}_n \in \mathscr{S}(\mathbb{R}^{4n})\}$ and proved that the postulates guarantee that the $\mathscr{W}_n$ arise as the Wightman distributions of a unique field theory satisfying the Gårding–Wightman axioms and that conversely the postulates hold in any Wightman field theory. This **reconstruction theorem** appeared in his paper "Quantum field theory in terms of vacuum expectation values," *Phys. Rev.* **101** (1956), 860–866, and is further discussed in Chapter XVII. Wightman's paper did not contain a translation of the axiom of uniqueness of the vacuum to properties of the $\mathscr{W}_n$. This was later added due to work of K. Hepp, R. Jost, D. Ruelle, and O. Steinmann, "Necessary conditions on Wightman functions," *Helv. Phys. Acta* **34** (1961), 542–544, and H. Borchers, "On the structure of the algebra of field observables," *Nuovo Cimento* **24** (1962), 214–236.

A second reformulation of the Wightman axioms is in terms of the **Schwinger functions**, that is the restriction of the Wightman functions to those points in the permuted forward extended tube (i.e., the union of the extended forward tube and its images under permutation of the x-space coordinates) which have purely real spatial coordinates and purely imaginary time coordinates. This reformulation is connected with the Euclidean approach to field theory which we discuss below, so we temporarily defer the historical notes on its development. Axioms on the Schwinger functions equivalent to the Wightman axioms can be found in K. Osterwalder and R. Schrader, "Axioms for Euclidean Green's functions, I," *Comm. Math. Phys.* **31** (1973), 83–112; II, (to appear).

Finally, there are axiom schemes which involve as fundamental structures objects that are distinct from purely local fields. One version emphasizes the role of "asymptotic fields" and thereby makes a direct connection with scattering theory. This is the LSZ axiom scheme of H. Lehmann, K. Symanzik and W. Zimmerman, "Zur Formulierung Quantisierter Feldtheorien," *Nuovo Cimento* **1** (1955), 205–225, "On the formulation of quantum field theories, II," *Nuovo Cimento* **6** (1957), 319–333. As a consequence of the machinery of Haag–Ruelle scattering theory (see Section XII.15), K. Hepp proved that a version of the LSZ axioms holds in any Wightman theory which is supplemented by suitable additional hypotheses on the mass spectrum. See K. Hepp, "On the connection between the LSZ and Wightman quantum field theory," *Comm. Math. Phys.* **1** (1965), 95–111, and his article in *Axiomatic Field Theory* (Brandeis Summer Institute, 1965), Gordon and Breach, New York, 1966.

A second approach to local quantum axiomatics involves the use of Banach algebras. Von Neumann first suggested the use of algebras of bounded operators to axiomatize quantum mechanics and developed much of theory of W^*-algebras ("von Neumann algebras") for this purpose. His work was clarified and expanded by I. Segal in "Postulates for general quantum mechanics," *Ann. Math.* **48** (1947), 930–947. Throughout the fifties Segal championed an algebraic approach to the problems in field theory and in 1964, R. Haag and D. Kastler formulated a set of axioms in "An algebraic approach to quantum field theory," *J. Math. Phys.* **5** (1964), 848–861; see also, H. Araki, "Local quantum theory, I," in *Local Quantum Theory* (R. Jost, ed.), Academic Press, New York, 1969. The relationship between the Haag–Kastler axioms and the Wightman axioms is not direct. *If* the fields in the Wightman axioms are self-adjoint, then one can form a family of algebras out of their spectral projections, but it is not clear that they satisfy the Haag–Kastler axioms for technical reasons, e.g., the commutation of fields in the Wightman sense might not imply commutation of the spectral projections (see Section VIII.5). Conversely, it is not clear how to reconstruct the fields from the Haag–Kastler local algebras. Nevertheless, the two sets of axioms are closely related and one expects them both to hold in reasonable models. This has been the case in the two-dimensional models constructed so far. We discuss the algebraic approach to field theory in Chapter XIX.

A third approach involves the analytic continuation to imaginary time where the Poincaré group is replaced by the Euclidean group. On the level of perturbation theory, this goes back to F. Dyson, "The S-matrix in quantum electrodynamics," *Phys. Rev.* **75** (1949), 1736–1755; and on the level of Wightman functions to Wightman's 1956 paper and the Hall–Wightman paper discussed below. It is at this level of continuation of Wightman functions that the Osterwalder–Schrader axioms operate. But there is a level which is probably more specialized in that it does not follow from only the Wightman axioms, in which one looks for Euclidean *fields*, i.e., operators whose expectation values are the Schwinger functions. Such an approach was first advocated by J. Schwinger, "On the Euclidean structure of relativistic field theory," *Proc. Nat. Acad. Sci. U.S.A.* **44** (1958), 956–965, and T. Nakano, "Quantum field theory in terms of Euclidean parameters," *Progr. Theoret. Phys.* **21** (1959), 241–259. The connection of this formulation with probabilistic ideas, such as the Feynman–Kac formula of Section X.10, and with classical statistical mechanics was first emphasized by K. Symanzik in "Euclidean quantum fields, I, equations for a scalar model," *J. Math. Phys.* **7** (1966), 510–525, and in "Euclidean quantum field theory" in *Local Quantum Theory* (R. Jost, ed.), Academic Press, New York, 1969. Subsequently, E. Nelson, in "Construction of Quantum Fields from Markoff Fields," *J. Functional Analysis* **12** (1973), 97 112, proposed a set of axioms defining a Euclidean field theory and showed that from any such theory, one could construct a quantum field theory satisfying the Wightman axioms. The converse problem of what must be added to the Wightman axioms to enable one to construct a Euclidean theory obeying all Nelson's axioms has not been definitely solved but a partial solution can be found in B. Simon, "Positivity of the Hamiltonian semigroup and the construction of Euclidean region fields," *Helv. Phys. Acta* **46** (1974), 686–696. This paper includes an example obeying the analogue of the Wightman axioms in one space–time dimension but *not* obeying Nelson's axioms, which shows some additional structure is present in Euclidean field theories.

The Bargmann–Hall–Wightman theorem appeared in D. Hall and A. Wightman, "A theorem on invariant analytic functions with applications to relativistic quantum field theory," *Mat.-Fys. Medd. Danske Vid. Selsk.* **31** (1957), 1–41. V. Bargmann's name is attached to the theorem because of the contributions he made to its proof.

A precursor of the PCT theorem was proven in G. Lüders, "On the equivalence of invariance under time reversal and under particle–antiparticle conjugation for relativistic field theories," *Danske Vid. Selsk. Mat.-Fys. Medd.* **28** (1954), 1–17. The PCT theorem itself was proven in W. Pauli, "Exclusion principle, Lorentz group, and reflection of space-time and charge," in *Niels Bohr and the Development of Physics* (W. Pauli, ed.) Pergamon Press, Oxford, 1955, and R. Jost, "Eine Bemerkung zum CTP Theorem," *Helv. Phys. Acta* **30** (1957), 409–416. For a discussion of the physical significance of the PCT theorem, see S. Gasiorowicz, *Elementary Particle Physics*, Wiley, New York, 1966, pp. 508–519.

The representation of the two-point function given in Theorem IX.34 is called the Källen–Lehmann representation because it was discovered by H. Umezawa and S. Kamefuchi in "The Vacuum in Quantum Electrodynamics," *Progr. Theoret. Phys.* **6** (1951), 543–558. See also G. Källen, "On the definition of the renormalization constants in quantum electro-

dynamics," *Helv. Phys. Acta* **25** (1952), 417–434, and H. Lehmann, "Über Eigenschaften von Ausbreitungsfunktionen und Renormierungskonstanten quantisierter Felder," *Nuovo Cimento* **11** (1954), 342–357.

It is clear from Section IX.8 that the problem of calculating the holomorphy envelopes of the permuted forward tube, the "primitive domain" for the n-point functions is important. For the three-point function, see G. Källen and A. S. Wightman, "The analytic properties of the vacuum expectation values of a product of three scalar local fields," *Mat.-Fys. Skr. Danske Vid. Selsk.* **1** (1958). For a general discussion of analyticity and quantum field theory, see A. S. Wightman, "Quantum field theory and analytic functions of several complex variables," *J. Indian Math. Soc.* **24** (1960), 625–677, or H. Epstein, "Some analyticity properties of the scattering amplitude in quantum field theory," in *Axiomatic Field Theory* (Brandeis Summer Institute, 1965), Gordon and Breach, New York, 1966.

Finally, let us briefly describe the role of "spin" in field theory and the resulting modification of the axioms to accommodate "spinor fields." To explain one of the subtleties associated with spin, we must return to our discussion of dynamics in the notes to Section VIII.11. There, dynamics is described a priori, not by unitary operators, U_t obeying $U_{t+s} = U_t U_s$ but by automorphisms of the states α_t obeying $\alpha_{t+s} = \alpha_t \alpha_s$. It is a theorem that every such automorphism which is a square of some other automorphism is induced by a unitary U unique up to an overall phase transformation $U \to e^{i\theta}U$. Thus U_t can be chosen so that U_t induces α_t and then, by uniqueness up to phase, $U_{t+s} = \lambda(t, s)U_t U_s$ where $\lambda(t, s)$ is a phase factor. In the case of dynamics where the group is $\mathbb{R}$, we can always find $\mu(t)$ with $\lambda(t, s) = \mu(t+s)\mu(t)^{-1}\mu(s)^{-1}$ so that $V(t) = \mu(t)U(t)$ obeys $V(t+s) = V(t)V(s)$. An analysis similar to this works for the Poincaré group but only up to a point. One indeed obtains a strongly continuous map of $\mathscr{L}_+^\uparrow$ into the unitaries obeying $U(AB) = \lambda(A, B)U(A)U(B)$ where $\lambda(A, B)$ is a phase factor. But it is no longer possible, in general, to obtain a strict representation by the substitution $V(A) = \mu(A)U(A)$ for suitable μ. Rather one has the following situation:

There is a group, $SL(2, \mathbb{C})$, and a two-to-one map Λ of $SL(2, \mathbb{C})$ onto $\mathscr{L}_+^\uparrow$. One forms a group $InSL(2, \mathbb{C})$ from $\mathbb{R}^4$ and $SL(2, \mathbb{C})$ by taking $InSL(2, \mathbb{C}) = SL(2, \mathbb{C}) \times \mathbb{R}^4$ in the set equality sense with group operation

$$\langle A, a\rangle\langle B, b\rangle = \langle AB, a + \Lambda(A)b\rangle$$

Thus the map $\tilde{\Lambda}$: $\langle A, a\rangle \to \langle \Lambda(A), a\rangle$ is a two-to-one map of $InSL(2, \mathbb{C})$ to $\mathscr{P}_+^\uparrow$. The basic theorem is that given a map $\tilde{U}$ from $InSL(2, \mathbb{C})$ to the unitaries with $\tilde{U}(AB) = \lambda(A, B) \times \tilde{U}(A)\tilde{U}(B)$, we can find $\mu(\cdot)$ on $InSL(2, \mathbb{C})$ so that $\tilde{V}(A) = \mu(A)\tilde{U}(A)$ obeys $\tilde{V}(AB) = \tilde{V}(A)\tilde{V}(B)$. Given U, a representation up to phase of $\mathscr{P}_+^\uparrow$, we can then define $\tilde{U}$ on $InSL(2, \mathbb{C})$ by $\tilde{U}(A) = U(\tilde{\Lambda}(A))$ and thus associate with U a representation of $InSL(2, \mathbb{C})$. This reduction is due to Bargmann and Wigner in the papers quoted in (4) of our discussion of dynamics in the notes to Section VIII.11; see also Chapter XIV.

Let 1 and -1 be the two elements of $SL(2, \mathbb{C})$ which go into the unit element of $\mathscr{L}_+^\uparrow$ under Λ (in fact, $SL(2, \mathbb{C})$ is the group of all 2×2 complex matrices with determinant 1 and the matrices, 1, -1 go into the unit of $\mathscr{L}_+^\uparrow$ when one defines $\Lambda(A)$ by $\Lambda(A)_{\mu\nu} = \mathrm{tr}(\sigma_\mu A \sigma_\nu A^{-1})$ where $\sigma_0 = 1$ and σ_i are the Pauli matrices). Then an irreducible representation, V, of $InSL(2, \mathbb{C})$ is always one of two types: either $V(-1) = 1$ or $V(-1) = -1$. These types are usually referred to respectively as the integral spin and half-integral spin cases, since in the two cases, the eigenvalues of the angular momentum operator J_z, the infinitesimal generator of the subgroup of $SL(2, \mathbb{C})$ which goes into rotations about the z axis are respectively $0, \pm 1, \pm 2, \ldots$ or $\pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \ldots$. We note that it is natural to extend the analysis of irreducible representations of $InSL(2, \mathbb{C})$ further to a complete set of invariants, namely the mass and the

"spin" (see, e.g., Wigner's paper), but we will only need this $V(-1) = \pm 1$ classification below. We also note that the integral spin cases are precisely those where the representation of $InSL(2, \mathbb{C})$ yields a representation of $\mathscr{P}_+^\uparrow$ rather than just a representation up to a factor.

Next, we define spinor fields, temporarily deferring the discussion of their connection with spin. Let $S(\cdot)$ be a *finite-dimensional* (of necessity not unitary!) irreducible representation of $SL(2, \mathbb{C})$, on a space of dimension d. A **spinor field of type S** is an object obeying the axioms stated for a Hermitian scalar field, with five changes:

(1) The single field $\varphi(\cdot)$ is replaced by a d-tuple of fields $\langle \varphi_1(\cdot), \ldots, \varphi_d(\cdot)\rangle$.
(2) The field $\varphi(f)$, with f real, is not required to be symmetric.
(3) The transformation law, Property 6, is replaced by

$$U(\Lambda, a)\varphi_i(x)U(\Lambda, a)^{-1} = \sum_{j=1}^{d} S(A^{-1})_{ij}\varphi_j(\Lambda x + a)$$

where $\Lambda = \Lambda(A)$.

(4) The vacuum is only required to be cyclic for

$$\{\varphi_1(f), \ldots, \varphi_d(f), \varphi_1^*(f), \ldots, \varphi_d^*(f) \mid f \in \mathscr{S}(\mathbb{R}^4)\}$$

(5) The relation $\varphi(f)\varphi(g) - \varphi(g)\varphi(f) = 0$ if f and g are spacelike separated is replaced by either:

(a) (Böse statistics)

$$\varphi_i(f)\varphi_j(g) - \varphi_j(g)\varphi_i(f) = 0$$
$$\varphi_i^*(f)\varphi_j(g) - \varphi_j(g)\varphi_i^*(f) = 0$$

or

(b) (Fermi statistics)

$$\varphi_i(f)\varphi_j(g) + \varphi_j(g)\varphi_i(f) = 0$$
$$\varphi_i^*(f)\varphi_j(g) + \varphi_j(g)\varphi_i^*(f) = 0$$

Depending on whether $S(-1) = 1$ or $S(-1) = -1$, we refer to integral or half-integral spin spinor fields. One has the remarkable

Theorem (spin and statistics theorem) Let $\{\varphi\}$ be a field of type S. Then, if φ obeys Bose statistics, S has integral spin, and if φ obeys Fermi statistics, S has half-integral spin.

The spin and statistics theorem for free fields appeared in M. Fierz, "Über die relativistische Theorie kräftfreirer Teilchen mit beliebigem Spin," *Helv. Phys. Acta* **12** (1939), 3–37, and W. Pauli, "On the connection between spin and statistics," *Phys. Rev.* **58** (1940), 716–722. For the general case, see G. Lüders and B. Zumino, "Connection between spin and statistics," *Phys. Rev.* **110** (1958), 1450–1453, and N. Burgoyne, "On the connection of spin with statistics," *Nuovo Cimento* **8** (1958), 607–609. When one has a theory with several different fields the relation of the spins to the commutation relations is somewhat complicated; see the Streater-Wightman book and G. F. Dell'antonio, "On the connection of spin with statistics," *Ann. Phys.* **16** (1961), 153–157.

There is also a PCT theorem for spinor fields. The PCT operator Θ acts on the fields by

$$\Theta\varphi_i(x)\Theta^{-1} = \sum_{j=1}^{d} A_{ij}\varphi_j^*(-x)$$

where A is an explicit matrix depending only on S. For a discussion, see the PCT papers quoted above or the Streater–Wightman book.

There has also been some discussion of "infinite spin fields," i.e., fields where $S(A)$ is replaced by some *infinite* dimensional representation of $SL(2, \mathbb{C})$. One difficulty with such fields is that the Bargmann–Hall–Wightman and PCT theorems may fail for them. See A. Oksak and I. Todorov, "Invalidity of the TCP-theorem for infinite-component fields," *Comm. Math. Phys.* **11** (1968), 125–130.

Finally, let us say a word about the connection between spinor fields and the spin of particles. "Particles" enter field theory as eigenstates of the "mass" operator $M = \sqrt{H^2 - \mathbf{P}^2} \equiv (\tilde{P} \cdot P)^{1/2}$. The subspace $\mathscr{H}_m = \{\psi \,|\, M\psi = m\}$ is left invariant by $InSL(2, \mathbb{C})$ and the representation of $InSL(2, \mathbb{C})$ on $\mathscr{H}_m$ is a direct sum of irreducibles. If there is a single irreducible summand, we say there is only one particle of mass m and its spin is the invariant associated to the representation. In general, there is only a tenuous connection between the "spin" in the S describing the spinor field and the spin of the particles of a theory. However, one critical connection remains: If $\varphi_1, \ldots, \varphi_k$ are fields (not necessarily in the same multiplets and not necessarily distinct), then $\varphi_1(f_1) \cdots \varphi_n(f_n)\psi_0$ can "couple" to one particle states (i.e., is not orthogonal) of half-integral spin (respectively, integral spin) only if an odd number of φ_i's (respectively, even number) are half integral spin. This allows one to relate the physical spin of a particle to its statistics. Other than this one connection, one can say almost nothing, for there can be more particles than fields, or more fields than particles or particles whose spins are unrelated to the spins of the fields (all these phenomena occur with suitably modified free fields based on the simple model of Section X.7).

Section IX.9 The ideas and proof in this section go back to the work of E. Gagliardo, "Caratterizzazioni delle trace sulla frontiera relative ad alcune classi di funzioni in n variabli," *Rend. Sem. Mat. Univ. Padova* **27** (1957), 284–305, and N. Aronszajn and K. Smith, "Theory of Bessel Potentials, I," *Ann. Inst. Fourier (Grenoble)* **11** (1961), 385–475. For a more detailed discussion of the restriction problem, see E. Stein, *Singular Integrals and Differentiability Properties of Functions*, Princeton Univ. Press, Princeton, New Jersey, 1970, Chapter VI.

The restriction results we discuss hold for flat or curved submanifolds. Much more subtle are a class of results which only hold for curved submanifolds. For example, if $f \in L^p(\mathbb{R}^2)$ with $p < \frac{4}{3}$, then $\hat{f}$ may be restricted to an L^2 function on the unit circle (but, if $p > 1$, it may not be possible to restrict it to a piece of coordinate axis). This result and the extensions appear in C. Fefferman, "Inequalities for Strongly Singular Convolution Operators," *Acta Math.* **124** (1970), 9–36.

The geometric measure which we referred to immediately before Theorem IX.39 is a generalization of arc length measure for curves. Intuitively, it is described as follows: At any point $x \in M$, choose an orthonormal set of tangent vectors to M at x and take the Lebesgue measure on the tangent space with respect to these coordinates. Then the measure of a very small set about x is approximately the Lebesgue measure of its normal projection onto the tangent space. In the usual differential geometric language, this is the measure on M associated with the metric on M induced by the natural metric on $\mathbb{R}^n$.

Section IX.10 The elaborate machinery of wave front sets and oscillatory integrals was developed in order to study partial differential operators and not merely for the modest problem of defining products of distributions. We have presented our discussion as an introduction to this machinery. Our treatment is closely patterned on parts of L. Hörmander, "Fourier integral operators, I" *Acta Math.* **127** (1971), 79–183. This paper introduced the notion of wave front set and originally defined it by using pseudo-differential operators (see below). It is a

proposition in Hörmander's paper that his definition is equivalent to the one we use. Notions similar to wave front set can be found in M. Sato, "Hyper-functions and partial differential equations," *Conference on Functional Analysis and Related Topics*, Swets and Zeitlinger, Tokyo, 1969, pp. 91–94. Detailed applications of wave front sets and oscillatory integrals to partial differential equations can be found in J. Duistermaat and L. Hörmander, "Fourier integral operators, II," *Acta Math.* **128** (1972), 183–269.

Fourier integral operators are the natural outgrowth of several lines of development. Pseudo-differential operators arise naturally as a generalization of partial differential operators with nonconstant coefficients. Let $a_i \in C^\infty(\Omega)$, $\Omega \subset \mathbb{R}^n$ and let p_i be a homogeneous polynomial of degree i. Then, for all $\varphi \in C_0^\infty(\Omega)$

$$\sum_{i=1}^{N} a_i(x)p_i(-iD)\varphi(x) = \sum_{i=1}^{N} a_i(x)\widecheck{(p_i(\theta)\hat{\varphi}(\theta))}$$

$$= (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{ix\cdot\theta} \left(\sum_{i=1}^{N} a_i(x)p_i(\theta) \right) \hat{\varphi}(\theta)\, d\theta$$

Since p_i is a polynomial of degree i, $\sum_{i=1}^{N} a_i(x)p_i(\theta)$ is a symbol of order N. If we replace $\sum_{i=1}^{N} a_i(x)p_i(\theta)$ by an arbitrary symbol of order N, the corresponding operator

$$(A\varphi)(x) = \int_{\mathbb{R}^n} e^{ix\cdot\theta} a(x, \theta)\hat{\varphi}(\theta)\, d\theta$$

is called a **pseudo-differential operator** of order N. A systematic calculus for such operators was developed in J. Kohn and L. Nirenberg, "On the algebra of pseudo-differential operators," *Comm. Pure Appl. Math.* **18** (1965), 269–305.

Pseudo-differential operators of order zero are called **singular integral operators**. Such operators arose in the classical technique of reducing a boundary value problem for an elliptic operator in a region Ω to an integral equation problem on $\partial\Omega$ (see the example in Section VI.5). For a discussion of these techniques see, for example, L. Hormander, "Pseudo-differential operators and non-elliptic boundary value problems," *Ann. Math.* **83** (1966), 129–209, or R. Seeley, "Elliptic singular integral equations," in *Singular Integrals, Proc. Symp. Pure Math.*, Amer. Math. Soc., Providence, Rhode Island, 1967, 308–315, where a detailed historical review is given.

For nonelliptic equations, it is quite natural to replace $x \cdot \theta$ by a more general phase function and such a procedure was followed by a variety of authors before Hörmander's systematic developments: P. D. Lax, "Asymptotic solutions of oscillatory initial value problems," *Duke J. Math.* **24** (1957), 627–646; D. Ludwig, "Exact and asymptotic solutions of the Cauchy problem," *Comm. Pure Appl. Math.* **13** (1960), 473–508; V. P. Maslov, *Theory of Perturbations and Asymptotic Methods*, Moskov. Gos. Univ., Moscow, 1965 (in Russian; French translation by J. Lascoux and R. Senor published by Dunod, Paris, 1972); G. I. Eskin, "The Cauchy problem for hyperbolic systems in convolutions," *Mat. Sb.* **74** (1967), 262–297; Yu. V. Egorov, "On canonical transformations of pseudo-differential operators," *Usp. Mat. Nauk.* **25** (1969), 235–236; and L. Nirenberg and F. Trèves, "On local solvability of linear partial differential equations, Parts I, II, *Comm. Pure Appl. Math.* **23** (1970), 1-38; 459 510. In particular, Maslov's book contains ideas which have been crucial in further developments.

Wave front sets are especially useful in discussing regularity (and nonregularity) of solutions of partial differential equations. For example, one has the following generalization of the elliptic regularity theorem (see, e.g., Fourier integral operators, II):

Theorem Let $P(x, D) = \sum_{|\alpha| \le n} a_\alpha(x) D^\alpha$ be a partial differential operator with C^∞ coefficients and let f be a C^∞ function. If $T \in \mathscr{D}'_{\mathbb{R}^n}$ solves $P(x, D)T = f$, then

$$WF(T) \subset \left\{ \langle x, k \rangle \;\middle|\; \tilde{P}(x, k) \equiv \sum_{|\alpha| = n} a_\alpha(x) k^\alpha = 0 \right\} \tag{IX.66}$$

There is a further refinement of this theorem which asserts that if a point (x_0, k_0) in the set on the right-hand side of (IX.66) lies in $WF(T)$, then automatically an entire associated set (the bicharacteristic strip with initial point (x_0, k_0)) lies in $WF(T)$. This refined theory goes under the name "propagation of singularities" and has its roots in geometrical optics.

Example 1 was shown to us by O. E. Lanford, III.

Theorem IX.44f has a natural translation if we consider distributions on a manifold M. It asserts that $WF(T)$ is a subset of the cotangent bundle of M.

Theorem IX.46 has an application to the problem of restricting a distribution to an embedded submanifold, a problem which we discussed from a different point of view in Section IX.9. Let us consider the case of an embedded curve in $\mathbb{R}^n$; for the general case, see Hörmander's paper: "Fourier integral operators, I," Theorem 2.5.11. Let $F: \mathbb{R} \to \mathbb{R}^n$ be an injective C^∞ function obeying: (i) grad $F(t) \neq 0$ for any t; (ii) $\lim_{t \to \pm\infty} |F(t)| = \infty$ (F is called a regularly embedded, proper, simple, smooth curve). Any function $g \in C_0^\infty(\mathbb{R}^n)$ has a "restriction" to the curve F, to wit $F_*(g)(t) = g(F(t))$. Now let $T \in \mathscr{D}'(\mathbb{R}^n)$. Can we find a natural meaning to $F_*(T)$, at least for some set of $T \in \mathscr{D}'(\mathbb{R}^n)$? To do this, we rephrase the definition of $F_*(g)$. Given $f \in C_0^\infty(\mathbb{R})$, let $f\delta_F$ be the distribution in $\mathscr{D}(\mathbb{R}^n)$ given by

$$(f\delta_F)(g) = \int_{-\infty}^{\infty} f(t) g(F(t))\, dt$$

If we think of $F_*(g)$ as a distribution, then

$$F_*(g)(f) = (f\delta_F)(g)$$

More to the point, if we pick a function $\chi \in C_0^\infty(\mathbb{R}^n)$ identically one in a neighborhood of $\{F(t) | t \in \operatorname{supp} f\}$, then

$$F_*(g)(f) = [g(f\delta_F)](\chi) \tag{IX.67}$$

where $g(f\delta_F)$ denotes the product of g and the distribution $f\delta_F$. If $WF(T) \oplus WF(f\delta_F)$ is disjoint from $\{\langle x, 0 \rangle\}$, then we can use (IX.67) to define $F_*(T)$! Thus, we must find $WF(f\delta_F)$. A simple argument (Problem 67) shows that $WF(\delta_F) = \{\langle x, k \rangle | x = F(t); k \cdot \text{grad } F = 0, k \neq 0\}$, the **normal bundle** $N(F)$ to the curve F and that $WF(f\delta_F) \subset WF(\delta_F)$. Thus, by Theorem IX.46, we have:

Theorem If $T \in \mathscr{D}'(\mathbb{R}^n)$ has its wave front set disjoint from the normal bundle $N(F)$, then $F_*(T)$ can be defined by (IX.67) and moreover

$$WF(F_*(T)) \subset F^*(WF(T)) \equiv \{\langle t, \text{grad } F \cdot k \rangle \mid \langle F(t), k \rangle \in WF(T)\}$$

PROBLEMS

1. Find the Fourier transform of $3x^2 + 1$.

†2. Give the details of the convergence of the Riemann sum to the integral at the end of the proof of Theorem IX.1.

3. (a) Let R be a rotation and R^t its transpose. Let $f \in \mathscr{S}$. Prove that $\widehat{f \circ R} = \hat{f} \circ R^t$.
   (b) Let D_λ be the map $D_\lambda x = \lambda x$ on $\mathbb{R}^n$. Let $f \in \mathscr{S}(\mathbb{R}^n)$. Prove that

$$\widehat{f \circ D_\lambda} = \lambda^{-n} \hat{f} \circ D_{\lambda^{-1}}$$

   (c) Let $T \in \mathscr{S}'(\mathbb{R}^n)$. Prove that

$$\widehat{(T \circ R)} = \hat{T} \circ R^t, \qquad \widehat{T \circ D_\lambda} = \lambda^{-n} \hat{T} \circ D_{\lambda^{-1}}$$

4. Compute the Fourier transform of $\mathscr{P}(1/x)$, the Cauchy principle part, by using Equation (V.4).

5. Compute the Fourier transform of $f(x) = e^{-\alpha x^2/2}$ as follows:
   (a) Prove that $-\lambda \hat{f}(\lambda) = \alpha\, d\hat{f}(\lambda)/d\lambda$ and conclude that $\hat{f}(\lambda) = ce^{-\lambda^2/2\alpha}$
   (b) Use the Plancherel theorem to prove $c = 1/\sqrt{\alpha}$.
   (c) Check the Fourier inversion formula explicitly in this example.

6. Let $\mathscr{H} = L^2(\mathbb{R}, e^{-x^2}\, dx)$ and define $\psi_n = x^n \in \mathscr{H}$ for $n = 0, 1, \ldots$.
   (a) Prove that $\sum_{m=0}^{M} ((ik)^m/m!)\psi_m \xrightarrow[M \to \infty]{} e^{ikx}$ in the norm topology on $\mathscr{H}$.
   (b) Suppose $\eta \in \mathscr{H}$ and $(x^m, \eta) = 0$ for all m. Prove $\varphi = 0$. (*Hint*: show that $\eta e^{-x^2} = 0$.)
   (b′) Reach the conclusion of (b) without recourse to the Fourier transform. (*Hint*: Use the fact that the functions $(x \pm i)^{-n}$ are total in $C_\infty(\mathbb{R})$ and the formula $(x + i)^{-1} = i \int_0^\infty e^{-s} e^{isx}\, ds$).
   (c) Let $\{H_n\}$ be the orthonormal set obtained from $\{\psi_n\}$ by Gram–Schmidt orthogonalization. Prove that $\{H_n\}$ is a basis for $\mathscr{H}$.
   (d) Prove that $\{H_n(x)e^{-x^2/2}\}_{n=0}^\infty$ is an orthonormal basis for $L^2(\mathbb{R}, dx)$.
   (e) Prove that $H_n(x)e^{-x^2/2}$ is just the nth Hermite function (defined in the Appendix to Section V.3).

7. Let $\{A_n(\lambda)\}$ be the polynomials determined by the formula

$$\sum_{n=0}^{\infty} A_n(\lambda) \frac{\alpha^n}{n!} = e^{-\alpha^2 + 2\alpha\lambda}$$

   Define $\phi_n(\lambda) = (2^n n!)^{-1/2} A_n(\lambda) e^{-\lambda^2/2}$.
   (a) Prove that

$$\phi_n(\lambda) = \frac{(-1)^n}{\sqrt{2^n n!}} e^{\lambda^2/2} \left(\frac{d}{d\lambda}\right)^n e^{-\lambda^2}$$

   so that the $\phi_n(\lambda)$ are just the Hermite functions of the Appendix to Section V.3.
   (b) If $f \in L^2(\mathbb{R}, dx)$ and $(f, \phi_n) = 0$ for all $n = 0, 1, \ldots$, prove that for all a,

$$\int f(x) e^{-(x-a)^2/2}\, dx = 0$$

   (c) Use the Fourier transform to show that if $\int_{\mathbb{R}} f(x) e^{-(x-a)^2/2}\, dx = 0$ for all a, then $f = 0$.
   (d) Conclude that $\{\phi_n\}$ is a basis for $L^2(\mathbb{R}, dx)$.

8. The purpose of this problem is to prove the Plancherel theorem and the inversion formula by using the Hermite functions. Let

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \qquad \text{and} \qquad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

(a) If $f \in \mathscr{S}(\mathbb{R}^n)$ prove $\widehat{A^\dagger f}(\lambda) = -i(A^\dagger \hat{f})(\lambda)$.
(b) Prove that $\hat{\phi}_n = (-i)^n \phi_n$.
(c) Supposing the fact that the Hermite functions are a basis for $L^2(\mathbb{R})$, prove the Plancherel theorem and the inversion formula.

9. Suppose that C is a continuous map of $\mathscr{S}(\mathbb{R}^n)$ into $C^\infty(\mathbb{R}^n)$ which commutes with translations. Prove that there is a $T \in \mathscr{S}'(\mathbb{R}^n)$ so that $C(\varphi) = T * \varphi$, for all $\varphi \in \mathscr{S}(\mathbb{R}^n)$. (*Hint*: If $T \in \mathscr{S}'(\mathbb{R}^n)$ and $\varphi \in \mathscr{S}(\mathbb{R}^n)$, then $T(\varphi) = (T * \tilde{\varphi})(0)$.)

10. Prove directly (without using the Fourier transform) that for fixed $f \in \mathscr{S}(\mathbb{R}^n)$, the map $g \mapsto f * g$ is a continuous linear transformation of $\mathscr{S}(\mathbb{R}^n)$ into $\mathscr{S}(\mathbb{R}^n)$.

11. Let μ_1 and μ_2 be finite Borel measures on $\mathbb{R}^n$ and define

$$(\mu_1 * \mu_2)(E) = \int_{\mathbb{R}^n} \mu_1(E - y)\, d\mu_2(y)$$

(a) Prove that $\mu_1 * \mu_2$ is a finite Borel measure on $\mathbb{R}^n$, that $\mu_1 * \mu_2 = \mu_2 * \mu_1$, and that for any $f \in C_\infty(\mathbb{R}^n)$

$$(\mu_1 * \mu_2)(f) = \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f(x + y)\, d\mu_1(x)\, d\mu_2(y)$$

(b) Prove that $\mu_1 * \mu_2$ is absolutely continuous with respect to Lebesgue measure if either μ_1 or μ_2 is absolutely continuous with respect to Lebesgue measure. Give an example where $\mu_1 * \mu_2$ is not absolutely continuous.

12. The Fourier transforms of Borel measures of mass one on $\mathbb{R}^n$ are sometimes called "characteristic functions." A characteristic function $E(\lambda)$ is said to be **infinitely divisible** if for all positive integers n, there exists a characteristic function $E_n(\lambda)$ so that $E(\lambda) = (E_n(\lambda))^n$.
(a) Let μ be a Borel measure of mass one on $\mathbb{R}$ and let E be the corresponding characteristic function. Prove that E is infinitely divisible if and only if for all n there is a Borel measure of mass one, μ_n, so that

$$\mu = \underbrace{\mu_n * \mu_n * \cdots * \mu_n}_{n \text{ times}}$$

(b) Show that

$$E(\lambda) = \exp(i\alpha\lambda - \tfrac{1}{2}\beta\lambda^2) + \int_{-\infty}^{\infty} (e^{i\lambda x} - 1)\, d\rho$$

is an infinitely divisible characteristic function if $\alpha \in \mathbb{R}$, $\beta \geq 0$, and ρ is a Borel measure of finite mass on $\mathbb{R}$. Give a (convolution) formula for the corresponding measure in terms of α, β, and ρ. What is the corresponding measure if $\rho = 0$? What is the corresponding measure if $\alpha = 0 = \beta$ and $\rho = \delta(x - x_0)$?

Remark: There is a characterization of the Fourier transforms of all infinitely divisible distributions known as the Lévy-Khinchin formula. See, for example, L. Breiman, *Probability*, Addison Wesley, Reading, Massachusetts, 1968, 193–195.

13. Let Ω be an open set in $\mathbb{R}^n$, K a compact subset of Ω. Prove that there is a function in $C_0^\infty(\Omega)$ which is equal to one on K. (*Hint*: See Problem 61 of Chapter V.)

14. The purpose of this exercise is to prove the Fourier inversion formula by an alternative method. Suppose that $f \in \mathscr{S}(\mathbb{R}^n)$.
(a) Prove that $\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} ((\sin x)/x)\, dx$ exists. Call it d. Now, show that

$$\lim_{\varepsilon \downarrow 0} \int_\varepsilon^{1/\varepsilon} \frac{\sin Rx}{x}\, dx = d \qquad \text{for any } R > 0$$

(*Hint*: Use facts about telescoping series.)
(b) Prove that

$$\int_0^\infty \left[\frac{f(y-u) + f(y+u)}{2} - f(y)\right] \frac{\sin Ru}{u}\, du \xrightarrow[R \to \infty]{} 0$$

(Use the Riemann–Lebesgue lemma.)
(c) Using (b) conclude that

$$4df(y) = \lim_{R \to \infty} \int_{-\infty}^{\infty} \left(\int_{-R}^{R} e^{i(y-x)\cdot k} f(k)\, dk\right) dx$$

(d) Prove that $f(y) = (\sqrt{2\pi}/4d) \int_{-\infty}^{\infty} e^{iky} \hat{f}(y)\, dk$.
(e) By letting $f(x) = e^{-x^2/2}$, conclude that $d = \pi/2$.

15. The purpose of this exercise is to provide an alternative proof of the Plancherel theorem.
(a) Prove directly that if $f, g \in \mathscr{S}(\mathbb{R}^n)$

$$\widehat{f * g} = (2\pi)^{n/2} \hat{f}\hat{g}$$

(b) Letting $\tilde{f}(x) = f(-x)$, prove that

$$(f * \bar{\tilde{f}})(y) = \int |\hat{f}(k)|^2 e^{iky}\, dk$$

(c) Set $y = 0$ and conclude that

$$\int |f(x)|^2\, dx = \int |\hat{f}(k)|^2\, dk$$

*16. Prove that the map $L^1(\mathbb{R}^n) \xrightarrow{\wedge} C_\infty(\mathbb{R}^n)$ is not onto by exhibiting a function in $C_\infty(\mathbb{R}^n)$ which is not in its range.

17. The purpose of this problem is to develop the Fourier transform on $L^1(\mathbb{R}^n)$ without reference to $\mathscr{S}(\mathbb{R}^n)$.
(a) If $f \in L^1(\mathbb{R}^n)$, prove directly that

$$\hat{f}(\lambda) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i\lambda x} f(x)\, dx$$

is a bounded continuous function. (*Hint*: Use the dominated convergence theorem.)

(b) If $f \in L^1(\mathbb{R}^n)$, prove that $\hat{f}(\lambda) \to 0$ as $|\lambda| \to \infty$. (*Hint*: Prove that $2\hat{f}(\lambda) = (2\pi)^{-n/2} \int e^{-ix\lambda}(f(x) - f(x - \pi\lambda/|\lambda|^2)\, dx$.

(c) Prove directly that $(2\pi)^{n/2}\hat{f}\hat{g} = \widehat{f * g}$.

18. Find a function $f(x)$ that satisfies all the conditions in the definition of "functions of positive type" except continuity. To which function of positive type is $f(x)$ equal a.e.?

19. Display a distribution of positive type that is not a function. What is its Fourier transform?

**20.* Prove the Bochner-Schwartz theorem (Theorem IX.10). (*Hint*: Mimic our proof of Bochner's theorem using the inner product $(\varphi, \psi) = T(\tilde{\overline{\varphi}} * \psi)$ and the formula $T(\tilde{\overline{\varphi}} * \varphi_x) = (T * \overline{\varphi} * \tilde{\varphi})(x)$.)

21. What does the generalization of the Paley–Wiener theorem to distributions with compact support say about the Fourier transform of distributions with support at the origin? Compute the same result directly by using Theorem V.11.

22. Let C be a convex, compact, balanced set in $\mathbb{R}^n$. Let

$$C^\circ = \{k \mid k \cdot x \geq -1 \text{ for all } x \in C\}$$

be its polar. Let ρ be the Minkowski functional of C°, i.e.,

$$\rho(\eta) = \sup_{x \in C}(\eta \cdot x) = \inf_{\lambda > 0}\{\lambda \mid \lambda \in \mathbb{R},\ \lambda\eta \in C^\circ\}$$

Prove the following version of the Paley–Wiener theorem:

A function $f \in \mathscr{S}(\mathbb{R}^n)$ has support in C if and only if $\hat{f}$ is the restriction to $\mathbb{R}^n$ of an entire function $\hat{f}(z)$ which obeys the condition that for any n there is a constant D_n so that

$$|\hat{f}(z)| \leq D_n(1 + |z|^2)^{-n} e^{-\rho(\operatorname{Im} z)}$$

23. Prove the extension of Theorem IX.16 in the case where $\Gamma_{a,\theta}$ is replaced with an arbitrary proper, open, convex cone Γ and

$$\Gamma^* = \{\eta \mid \eta \cdot x \geq 0 \text{ for all } x \in \Gamma\}$$

24. (a) Let f be a measurable function on a measure space $\langle M, \mu\rangle$. Let

$$m_f(t) = \mu\{x \mid |f(x)| > t\}$$

Prove that if $f \in L^p(M, d\mu)$, then

$$\int_M |f|^p\, d\mu = -\int_0^\infty t^p\, dm_f(t) \qquad \text{(Stieltjes integral)}$$

(b) Prove that if $f \in L^p(M, d\mu)$, then

$$m_f(t) \leq \|f\|_p^p t^{-p}$$

(c) Prove that $f \in L^p(M, d\mu)$ if and only if

$$\int_0^\infty t^{p-1} m_f(t)\, dt < \infty$$

and in that case $\|f\|_p^p = p\int_0^\infty t^{p-1} m_f(t)\, dt$.

25. Prove that if $r < p < s$ and $f \in L^r_w \cap L^s_w$, then $f \in L^p$ and

$$\|f\|_p^p \leq \left(\frac{1}{p-r} + \frac{1}{s-p}\right)[\|f\|_{r,w}^r]^{(s-p)/(s-r)}[\|f\|_{s,w}^s]^{(p-r)/(s-r)}$$

26. (Hunt's interpolation theorem)

(a) Let $1 \leq p_0 < p_1 < \infty$, $0 < t < 1$, $p^{-1} = tp_1^{-1} + (1-t)p_0^{-1}$. Show that $f \in L^p_w$ if and only if there exists a C so that for $\lambda > 0$, f can be decomposed as $f = f_{0,\lambda} + f_{1,\lambda}$ with $f_{0,\lambda} \in L^{p_0}$, $f_{1,\lambda} \in L^{p_1}$ and

$$\|f_{0,\lambda}\|_{p_0} \leq C|\lambda|^{1-(p/p_0)}, \qquad \|f_{1,\lambda}\|_{p_1} \leq C|\lambda|^{1-(p/p_1)}$$

(*Hint*: Try $f_{0,\lambda}(x) = f(x)$ if $|f(x)| > \lambda$.)

(b) Prove that $\|f\|_{p,w} = C$, where C is the smallest constant which can be used in part (a).

(c) Use (a) and (b) to prove Hunt's interpolation theorem.

27. (a) Let $f \in L^p(M, d\mu)$. Prove that $t^p\mu\{x \mid |f(x)| > t\} \to 0$ as $t \to 0$ or ∞.

(b) Put a metric on $L^p_w(M, d\mu)$ by $\rho(f, g) = \|f - g\|_{p,w}$. Prove that $L^p(\mathbb{R}^n, dx)$ is not dense in $L^p_w(\mathbb{R}^n, dx)$ in this metric.

Note: In Hunt's theorem, T is defined on L^p_w not by a density argument (which does not work by the above) but by showing that if $f \in L^p_w$ for $p_0 < p < p_1$, then f can be written $f = f_0 + f_1$ with $f_0 \in L^{p_0}$ and $f_1 \in L^{p_1}$. Thus we can define $Tf = Tf_0 + Tf_1$.

†*28.* Fill in the details in the derivation of Sobolev's inequality (Example 3, Section 4).

29. Prove that the extension of the Fourier transform to $L^p(\mathbb{R}^n)$ given by the Hausdorff-Young theorem coincides with the restriction to $L^p(\mathbb{R}^n)$ of the Fourier transform on $\mathscr{S}'(\mathbb{R}^n)$.

30. (weak Hausdorff–Young) Prove that $\hat{f} \in L^q_w$ if $f \in L^p_w$ where $1 < p < 2$ and $p^{-1} + q^{-1} = 1$.

31. Prove Young's Theorem in the case $1 \leq p, q \leq 2$, $r \geq 2$ by using Hölder's inequality and the Hausdorff–Young theorem twice.

32. (weak Young theorem) Use the generalized Young inequality to prove that $f * g \in L^r_w$ if $f \in L^p_w$, $g \in L^q_w$ and $p^{-1} + q^{-1} = 1 + r^{-1}$, $1 < p, q, r < \infty$.

**33.* Provide a proof of Proposition 1 of the Appendix to Section IX.4 which does not use interpolation.

34. (a) Let $\|\cdot\|_0$ be the L^2 norm on $C_0^\infty(\mathbb{R}^n)$ and let $\|f\|_1 = \|f\|_0 + |f(0)|$. Show that $\|\cdot\|_0$ and $\|\cdot\|_1$ are not consistent. Compute the interpolation spaces X_t anyway.

(b) Let $X = C[0, 1]$. Define $\|f\|_0 = \int_0^1 |f(x)|\, dx$ and let $\|f\|_1 = \sum_{n=1}^\infty 2^{-n}|f(r_n)|$ where $\{r_n\}_{n=1}^\infty$ is an ordering of the rationals. Show that $\|f\|_+ = 0$ for all $f \in X$.

†*35.* Fill in the details of the proof that $X_t = \mathscr{H}_{m_t}$ in Example 3 of the Appendix to Section IX.4.

36. Suppose $\alpha \in \mathbb{R}$ and $p > 1$. Define H^p_α to be the completion of $C_0^\infty(\mathbb{R}^n)$ in the norm $\|\varphi\|_{\alpha,p} = \|((1 + k^2)^{\alpha/2}\hat{\varphi}\|_p$.

(a) Show that the norms $\|\cdot\|_{\alpha,p}$ are consistent.

(b) Let $p_0, p_1 > 1$ and $\alpha_0, \alpha_1 \in \mathbb{R}$ be fixed. Prove that the interpolating spaces X_t between $H^{p_0}_{\alpha_0}$ and $H^{p_1}_{\alpha_1}$ are equal to $H^{p_t}_{\alpha_t}$ for each $0 \leq t \leq 1$ where $p_t = tp_1^{-1} + (1-t)p_0^{-1}$ and $\alpha_t = t\alpha_1 + (1-t)\alpha_0$.

*37. Let X be a complex vector space with consistent norms $\|\cdot\|^{(0)}$ and $\|\cdot\|^{(1)}$. The purpose of this problem is to sketch the proof of the statement $X_t = \tilde{X}_t$ in the Appendix to Section 4. We use the notation introduced there.

(a) Show that if $x \in X_0 \cap X_1$, there exists $x_n \in X$ so that $x_n \to x$ in both the $\|\cdot\|^{(0)}$-norm and the $\|\cdot\|^{(1)}$-norm.

(b) Use (a) and the inequality

$$\|x\|_+ \leq \|x\|^{(t)} \leq \max\{\|x\|^{(0)}, \|x\|^{(1)}\}$$

to prove that it is sufficient to prove that $X_0 \cap X_1$ is dense in $\tilde{X}_t$ in order to conclude that $\tilde{X}_t = X_t$.

(c) Define $\mathscr{F}_\infty$ to be those $f \in \mathscr{F}$ such that

(i) $\|f(ia)\|^{(0)} \to 0$ as $a \to \pm\infty$

(ii) $\|f(1 + ia)\|^{(1)} \to 0$ as $a \to \pm\infty$

(iii) $\|f(z)\|_+ \to 0$ as $\operatorname{Im} z \to \pm\infty$ in the strip, uniformly in $\operatorname{Re} z$.

Prove that $\mathscr{F}_\infty/(\mathscr{F}_\infty \cap K_t) = \mathscr{F}(X)/K_t$.

(d) Suppose that $h \in \mathscr{F}(X)$ and $h(z) = h(z + ia)$ for all $z \in S$. Define

$$y_n(t) = a^{-1} \int_0^a e^{-2\pi(t+is)n/a} h(t + is)\, ds$$

Show that $y_n(t) = y_n$ is independent of t, $y_n \in X_0 \cap X_1$, and

$$\frac{1}{N} \sum_{m=1}^{N} \sum_{n=-m}^{m} y_n e^{2\pi i n z/a} \xrightarrow{\|\|\cdot\|\|} h(z)$$

where the convergence is uniform with respect to y in $\|\cdot\|^{(1)}$ for $z = 1 + iy$ and in $\|\cdot\|^{(0)}$ for $z = iy$.

(e) Show that the set of functions in $\mathscr{F}_\infty$ of the form $e^{\beta z^2}(\sum_{n=1}^{N} x_n e^{\alpha_n t})$ where $x_n \in X_0 \cap X_1$, with $\beta > 0$, α_n, and N arbitrary, is dense in $\mathscr{F}_\infty$. (*Hint*: Since $e^{2\beta z^2} f \xrightarrow{\beta \to 0} f$ we need only look at functions of the form $g = e^{2\beta z^2} f$. Let $h = e^{\beta z^2} f$ and show that

$$h_n(z) = \sum_{m=-\infty}^{\infty} h(t + inm)$$

is a well-defined periodic element of $\mathscr{F}(X)$. Then, use (d) and the statement $\lim_{n\to\infty} e^{\beta z^2} h_n = g$.)

(f) Conclude that $X_t = \tilde{X}_t$.

38. (a) Let $\{\varphi_n\}$ be an orthonormal set (not necessarily complete) in a Hilbert space $\mathscr{H}$. Show that if C is a compact operator on $\mathscr{H}$, then $\|C\varphi_n\| \to 0$.

(b) Let $F \in L^1(\mathbb{R}^n, dx)$ and define

$$(A\varphi)(x) = \int_{\mathbb{R}^n} F(x - y)\varphi(y)\, dy$$

Prove that A is not compact unless F is the zero function.

39. (a) Let $f \in L^p_w$; $g \in L^{p'}_w$ where $p^{-1} + (p')^{-1} = 1$. Suppose that q satisfies $q^{-1} + p^{-1} < 1$. Then for all $h \in L^q$, prove that

$$\|f(g * h)\|_q \leq C_{p,q} \|f\|_{p,w} \|g\|_{p',w} \|h\|_q$$

(b) Let $0 < s < n/q$. Let $|p|$ be the operator $\sqrt{-\Delta}$ on $L^q(\mathbb{R}^n)$. Show that $|x|^{-s}|p|^{-s}$ defines a bounded map of $L^q(\mathbb{R}^n)$ into itself.

40. Let $N(h, f)$ be the operator $g \to h(f * g)$ on $L^2(\mathbb{R}^n)$.

(a) Prove that $N(h, f) \in \mathscr{I}_2$ if $h, f \in L^2$, and $\|N(h, f)\|_{\mathscr{I}_2} \leq \|h\|_2 \|f\|_2$.

(b) Prove that $\|N(h, f)\|_{\text{op}} \leq \|h\|_p \|f\|_q$ if $p^{-1} + q^{-1} = 1$ and $p \geq 2$.

(c) Prove that $N(h, f)$ is compact if $h \in L^p$, $g \in L^q$, $2 \leq p < \infty$.

(d) If $f \in L^1 \cap L^2$, prove that $N(f, h) \in \mathscr{I}_p$ if $h \in L^p$, $2 \leq p < \infty$. (*Hint*: Use interpolation.)

†41. This problem outlines the complex variables argument in the Malgrange–Ehrenpreis theorem.

(a) Let $f(z)$ be an analytic function of one complex variable on the disk $|z| \leq 1$ and let $p(z) = a_m z^m + a_{m-1} z^{m-1} + \cdots + a_0$. Prove that

$$|a_0 f(0)| \leq (2\pi)^{-1} \int_0^{2\pi} |f(e^{i\theta}) p(e^{i\theta})|\, d\theta$$

(*Hint*: Let $q(z) = (\prod_j (\bar{z}_j z - 1)/(z - z_j))p(z)$ where the z_j are the zeros of f inside the unit circle. Notice that q is analytic on the disk and $|q(z)| = |p(z)|$ for $|z| = 1$.)

(b) Let f and p be as in part (a) and prove that

$$|a_k f(0)| \leq \frac{m!}{k!\,(m-k)!} (2\pi)^{-1} \int_0^{2\pi} |f(e^{i\theta}) p(e^{i\theta})|\, d\theta$$

(c) Let $F(\zeta)$ be an entire function of n complex variables and let $p(\zeta)$ be a polynomial of degree n. Suppose that $g(\zeta)$ is a nonnegative integrable function with compact support depending only on the absolute values $|\zeta_i|$, $i = 1, \ldots, n$. Prove that

$$|F(0) D^\alpha p(0)| \int_{\mathbb{C}^n} |\zeta|^\alpha g(\zeta)\, d\zeta \leq C_0 \int_{\mathbb{C}^n} |F(\zeta) p(\zeta)| g(\zeta)\, d\zeta$$

($d\zeta$ denotes Lebesgue measure on $\mathbb{C}^n$ and C_0 is a constant depending on α and m.)

(d) Use part (c) to prove the statement

$$|\tilde{q}(x)\hat{\varphi}(x)| \leq C_1 \int_{|\zeta| \leq \varepsilon} |\hat{\varphi}(x + \zeta) q(x + \zeta)|\, d\zeta$$

in the proof of the Malgrange–Ehrenpreis theorem.

Reference: K. Yosida, *Functional Analysis*, Springer, Berlin, 1965, pp. 185–186.

42. Find explicitly a fundamental solution for the ordinary differential equation $u'' = f$.

43. What do the regularity theorems of Section 6 say about the regularity of eigenfunctions of atomic Hamiltonians?

References: T. Kato, *Comm. Pure Appl. Math.* **10** (1957), 151–171; Section XIII.10 in Volume III of this series.

44. (a) Define the operation $\bar{\partial}$ on the C^∞ functions from $\mathbb{C}$ to $\mathbb{C}$ by $\bar{\partial} f = \partial f/\partial x + i\, \partial f/\partial y$ where $z \in \mathbb{C}$ is written $z = x + iy$. Prove that $\bar{\partial} f = 0$ is a restatement of the Cauchy–Riemann equations.

(b) Let $T \in \mathscr{D}'_{\mathbb{R}^2}$ where $\mathbb{C}$ is thought of as $\mathbb{R}^2$ and let $\bar{\partial} = \partial/\partial x + i\, \partial/\partial y$. Prove that if $\bar{\partial} T = 0$, then T is actually an analytic function. (*Hint*: Prove that $\Delta T = 0$ and apply the elliptic regularity theorem.)

(c) Let $T \in \mathscr{D}_{\mathbb{R}^{2n}}$ and suppose $\bar{\partial}_j T = 0$ for all $j = 1, 2, \ldots, n$. Prove that T is analytic.

45. (a) Prove that if Ω is a bounded open set and $V \in C^m(\Omega)$, $u \in W_k(\Omega)$ with $k \leq m$, then $Vu \in W_k(\Omega)$.

(b) Prove that if u is a weak solution of $-\Delta u + Vu = Eu$ and $V \in C^m(\Omega)$, then $u \in C^\ell(\Omega)$ for $\ell < m - \frac{1}{2}n + 2$.

*46. Using Sobolev's inequality (IX.19), prove the L^p Sobolev imbedding theorem; i.e. if $q^{-1} = p^{-1} - n\alpha^{-1}$ $(\alpha > 0,\ 1 < p, q < \infty)$ and if $f \in L^p$, then $g = \widehat{(1 + k^2)^{-\alpha} \hat{f}} \in L^q$.

47. Suppose that $f \in L^2(\mathbb{R}^3)$ and $\partial f/\partial x_i \in L^2(\mathbb{R}^3)$ for $i = 1, 2, 3$. Prove that $f \in L^p(\mathbb{R}^3)$ for all $p < 6$. (*Hint*: Use the Plancherel theorem, the function $(1 + |k|^2)^d$, and the Hausdorff–Young theorem.)

48. Let $\{f_\alpha\}_{|\alpha| \le m}$ be a family of $C^{|\alpha|}$ functions on $\mathbb{R}^n$. Let T and S be the differential operators

$$T\varphi = \sum_{|\alpha| \le m} \bar{f}_\alpha D^\alpha \varphi, \qquad S\varphi = \sum_{|\alpha| \le m} (-1)^{|\alpha|} D^\alpha (f_\alpha \varphi)$$

Let $T_{\min}$ denote the operator T defined on $C_0^\infty(\mathbb{R}^n)$ and let $T_{\max}$ be T defined on $\{\varphi \mid \varphi \in L^2(\mathbb{R}^n),\ T\varphi \in L^2(\mathbb{R}^n)\}$. Similarly, define $S_{\min}$ and $S_{\max}$.

(a) Prove that $S_{\min}^* = T_{\max}$, $T_{\min}^* = S_{\max}$.

(b) Prove that $T_{\min}$ is essentially self-adjoint if and only if both $T_{\min} = S_{\min}$ and $T_{\max}$ is self-adjoint.

Remark: When $T_{\min} = S_{\min}$, one says that T is *formally self-adjoint*. It may happen that $T_{\min}$ is formally self-adjoint but not even essentially self-adjoint, e.g. $-\Delta - x^4$ on $\mathbb{R}^n$. This is further discussed in the Appendix to Section X.1 and in Section X.5.

49. Let $H_n(x; \kappa) = \mathscr{F}^{-1}((\lambda^2 + \kappa^2)^{-1})$. Thus $G_0(x, y) = H_n(x - y; \kappa)$ is the free Green's function on $\mathbb{R}^n$. Suppose that $\kappa > 0$.

(a) Prove that $H_n(x; \kappa) = \kappa^{n-2} H_n(x\kappa; 1)$.

(b) Prove that

$$H_n(x; 1) = (4\pi)^{-n/2} \int_0^\infty e^{-\delta} e^{-|x|^2/4\delta} \frac{d\delta}{\delta^{n/2}} \tag{IX.68}$$

Hint: Use the form of the free propagator and the relation

$$(H_0 + 1)^{-1} = \int_0^\infty e^{-t} e^{-tH_0}\, dt$$

(c) Prove that $H(x; 1)$ is monotone decreasing in x and positive and that for $n \ge 3$,

$$H_n(x; 1) \le |x|^{2-n}$$

(d) If $n \ge 3$, prove that

$$\lim_{|x| \to 0} |x|^{n-2} H_n(x; 1) = (4\pi)^{-n/2} \int_0^\infty e^{-1/4y} \frac{dy}{y^{n/2}}$$

(*Hint for* (c) *and* (d): Let $y = \delta/|x|^2$.)

(e) Prove that $\lim_{|x| \to \infty} e^{|x|} |x|^{n/2 - 1/2} H_n(x; 1)$ exists and is nonzero. (*Hint*: Let $y = 2\delta/|x|$.)

50. (a) Let $T_\alpha = |x|^{-\alpha} \in \mathscr{S}'(\mathbb{R}^n)$ with $0 < \alpha < n$. Prove that $\hat{T}_\alpha$ is a C^∞ function on $\mathbb{R}^n \backslash \{0\}$ with $\hat{T} \circ R = \hat{T}$ for any rotation and $\hat{T} \circ D_\lambda = \lambda^{-n+\alpha} \hat{T}$ where D_λ is given in Problem 3. Conclude that

$$\widehat{|x|^{-\alpha}}(k) = C_{\alpha, n} |k|^{-n+\alpha}$$

(b) Let $T_{\alpha,\lambda} = (|k|^2 + \lambda^{-2})^{-\alpha/2}$, $0 < \alpha < n$, on $\mathbb{R}^n$. Prove that $\hat{T}_{\alpha,\lambda} \to \hat{T}_{\alpha,0}$ as $\lambda \to 0$ uniformly on compact subsets of $\mathbb{R}^n \backslash \{0\}$. Prove that $\hat{T}_{\alpha,\lambda} = \lambda^{-n+\alpha} \hat{T}_{\alpha,1} \circ D_{\lambda^{-1}}$ and conclude that $|k|^{n-\alpha} \hat{T}_{\alpha,1}(k)$ is bounded on the unit ball.

(c) Prove that $\hat{T}_{\alpha,1}(k)$ falls off exponentially and conclude that $\hat{T}_{\alpha,1}(k) \in L_w^{n/n-\alpha}$.

51. Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$ and let $\alpha > 0$. Prove that there is a constant $C_{\alpha,\varphi}$, so that

$$\sup_{|x| \le 1} \left| \left(\frac{x}{t}\right)^\alpha (e^{-iH_0 t} \varphi)(x) \right| \le C_{\alpha,\varphi}\, t^{-n/2} \qquad \text{for} \quad t > 1$$

Reference: J. Kupsch and W. Sandas: "Møller Operators for Scattering on Singular Potentials," *Comm. Math. Phys.* **2** (1966), 147–154.

52. Let $H_0 = -\Delta$ on $\mathbb{R}^n$.

(a) Prove that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash 0)$ if $n \ge 4$.

(b) Suppose that $n \le 3$ and $A = -\Delta \restriction C_0^\infty(\mathbb{R}^n \backslash 0)$. Let $\varphi = \widehat{(\lambda^2 - i)^{-1}}$. Prove that $\varphi \in D(A^*)$ and that $A^* \varphi = i\varphi$. Conclude that $-\Delta$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash 0)$ if $n \le 3$.

53. Use the Källen–Lehmann representation to prove that a quantum field $\varphi(x)$ cannot be a well-defined operator-valued *function* on $\mathbb{R}^4$. (*Hint*: Prove that $(\psi_0, \varphi(x)\varphi(y)\psi_0)$ is a bounded function, so that $\varphi(f)\psi_0 = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$, thus violating the cyclicity of ψ_0.)

54. Let $f_n \to f$ in $\mathscr{S}(\mathbb{R}^4)$. Let $\psi \in D$. Prove that properties 3 and 4 of Section IX.8 imply that $\langle f,\ g \rangle \mapsto \langle \psi,\ \varphi(f)\varphi(g)\psi \rangle$ is jointly continuous. Conclude from this that $\varphi(f_n)\psi \to \varphi(f)\psi$.

55. (a) Let $g \in C_0^\infty(\mathbb{R}^n)$, with $\int_{-\infty}^\infty g(x_1, x_2, \ldots, x_n)\, dx_1 = 0$ for each fixed $\langle x_2, \ldots, x_n \rangle \in \mathbb{R}^{n-1}$. Prove that $g = \partial h/\partial x_1$ for some $h \in C_0^\infty(\mathbb{R}^n)$.

(b) Let $T \in \mathscr{D}'(\mathbb{R}^n)$ with $T(x_1 + a, x_2, \ldots, x_n) = T(x_1, x_2, \ldots, x_n)$ for all a in the sense that $T(U_a f) = T(f)$ for all $f \in \mathscr{D}(\mathbb{R}^n)$ where $(U_a f)(x_1, \ldots, x_n) = f(x_1 - a, \ldots, x_n)$. Prove there exists $S \in \mathscr{D}'(\mathbb{R}^{n-1})$ with

$$T(x_1, x_2, \ldots, x_n) = S(x_2, \ldots, x_n)$$

in the sense that $T(f) = S(I_1(f))$ for all $f \in \mathscr{D}(\mathbb{R}^n)$ where $(I_1(f))(x_2, \ldots, x_n) = \int f(x_1, \ldots, x_n)\, dx_1$. (*Hint*: Choose $F \in \mathscr{D}(R)$ with $\int F(t)\, dt = 1$. Recall from Problem 47 of Chapter V that $\partial T/\partial x_1 = 0$. Finally use (a) to prove that

$$g = f - F(x_1) I_1(f) = \partial h/\partial x_1)$$

(c) Let T and S be as in (b). Prove that if T is tempered, then S is tempered.

56. The goal of this problem is to prove that any tempered distribution T with support in $\bar{V}_+ \cup (-\bar{V}_+)$ can be written $T = R + A$ where supp $R \subset \bar{V}_+$ and supp $A \subset -\bar{V}_+$.

(a) Let f be a C^∞ function on the unit sphere S in $\mathbb{R}^4$ with $f = 1$ on $\bar{V}_+ \cap S$ and $f = 0$ on $-\bar{V}_+ \cap S$. Let $\chi(\mathbf{x}) = f(\mathbf{x}/|\mathbf{x}|)$. Show that $(x^2)^n \chi(\mathbf{x})$ is a C^{2n-1} function.

(b) Suppose that $|T(g)| \le \sum_{|\alpha| \le N,\, |\beta| \le M} \|x^\alpha D^\beta g\|_\infty$. Prove that $(x^2)^{M+1} T$ can be written as $S_+ + S_-$ where supp $S_+ \subset \bar{V}_+$ and supp $S_- \subset -\bar{V}_+$. (*Hint*: Let $S_+(f) = T[(x^2)^{M+1} \chi f]$.)

(c) Pick a fixed h in $C_0^\infty(\mathbb{R}^4)$, with $h \equiv 1$ near $x = 0$. Let

$$Hf = (x^2)^{-M-1} \left[f - \sum_{|\beta| \le 2M+1} \frac{(D^\beta f)(0)}{\beta!}\, x^\beta h \right]$$

Prove that $T(f) = (x^2)^{M+1} T(Hf) + T_0$ where T_0 has support at the origin.

†57. Prove Theorem IX.38 for the case of codimension greater than one.

†58. Fill in the details of the proof of Theorem IX.40.

59. Give an example of a tempered distribution T given by a polynomially bounded C^∞ function F so that the family of translates $\{T_x\}$ is bounded as a family of distributions but such that F is *not* a bounded function. (*Hint*: Modify Example 1 of Section IX.10).

†60. Complete the proof of Theorem IX.43.

61. Let $T, S \in \mathscr{D}'(\mathbb{R})$ so that the products TS, $T'S$, and TS' all exist. Prove that $(TS)' = T'S + TS'$.

62. Let C be a convex cone in $\mathbb{R}^n$ with nonempty interior. Let $\mathscr{A}$ be the family of functions analytic in $\mathbb{R}^n + iC$, polynomially bounded at infinity and as $\operatorname{Im} z \downarrow 0$. For $F \in \mathscr{A}$, let $BV(F)$ denote the distributional boundary value of F. If $F, G \in \mathscr{A}$, prove that the product $BV(F)BV(G)$ exists and that

$$BV(F)BV(G) = BV(FG)$$

63. For any $T \in \mathscr{D}'(\mathbb{R}^n)$ and any $\alpha \in I_+^n$ prove that $WF(D^\alpha T) = WF(T)$.

64. (a) For any $T \in \mathscr{D}'(\mathbb{R}^n)$ and $f \in \mathscr{D}(\mathbb{R}^n)$, prove that

$$WF(fT) \subset \{\langle x, k\rangle \mid x \in \operatorname{supp} f; \langle x, k\rangle \in WF(T)\}$$

and that

$$WF(fT) \supset \{\langle x, k\rangle \mid f(x) \neq 0; \langle x,\ k\rangle \in WF(T)\}$$

(b) Give an example of f, T as in part (a) for which

$$WF(fT) \neq \{\langle x, k\rangle \mid x \in \operatorname{supp} f; \langle x, k\rangle \in WF(T)\}$$

*65. (a) Define the asymptotic conical support $ACS(T)$ of a distribution T as the complement of those $k \neq 0$ for which there exists a neighborhood N and a Λ_0 so that $\operatorname{supp} T \cap \lambda N = \varnothing$ if $\lambda > \Lambda_0$. Prove that $ACS(T)$ is a closed cone.
(b) Prove that for $T \in \mathscr{S}'(\mathbb{R}^n)$, $WF_x(T) \subset ACS(\hat{T})$ for any $x \in \mathbb{R}^n$.
(c) Without using the machinery of oscillatory integrals, obtain enough information about $WF(\Delta_+)$ to prove that the product $\theta\Delta_+$ exists.

66. †(a) Prove Theorem IX.46.
(b) Refine Theorem IX.46 by finding necessary and sufficient conditions on F, an asymptotic symbol of order k, so that $\operatorname{sing\,supp}(\hat{F}) = \varnothing$.

67. Define $\operatorname{Sym}(\Omega, s, m, \rho, \delta)$ as $\operatorname{Sym}(\Omega, s, m)$ was defined but with (IX.63) replaced by

$$|(D_x^\alpha D_\theta^\beta a)(x, \theta)| \leq d(1 + |\theta|)^{m - \rho|\beta| + \delta|\alpha|}$$

Extend Theorem IX.49 to the case $\delta < 1$, $\rho > 0$.

†68. Prove that

$$a(x, \theta; m) = (m^2 + |\theta|^2)^{-1/2} \exp(-ix_0[(m^2 + |\theta|^2)^{1/2} - |\theta|])$$

is an asymptotic symbol of order -1.

†69. Prove Lemmas 1 and 2 in the proof of Theorem IX.47.

†70. Prove that the map V used in the proof of Theorem IX.47 maps $\operatorname{Sym}(\Omega, s, m)$ continuously to $\operatorname{Sym}(\Omega, s, m - 1)$.

†71. Prove that $\langle a, f\rangle \to af$ is a continuous bilinear map of $\operatorname{Sym}(\Omega, s, m) \times C_0^\infty(\Omega)$ to $\operatorname{Sym}(\Omega, s, m)$.

†72. Complete the proof of (c) of Theorem IX.48. *Hint*: Show that

$$t^n \exp(i\omega(k)t) = \left[\frac{\omega(k)}{i|k|^2}(\mathbf{k} \cdot \nabla_k)\right]^n e^{i\omega(k, t)}$$

where $\omega(k) = \sqrt{m^2 + k^2}$.

†73. Under the situation described in the notes to Section IX.10, prove that $WF(f\delta_F) \subset N(F)$ and that $WF(\delta_F) = N(F)$.

†74. Find two distributions T, S of compact support so that TS exists but $\int \hat{T}(\ell)\hat{S}(k - \ell)\, d\ell$ diverges absolutely for all k.

†,*75. The purpose of this problem is to prove the change of variables formula in (f) of Theorem IX.44.
(a) Verify the formula when M is a linear transformation.
(b) Show that it is enough to prove that

$$WF_{x=0}(T \circ M) = WF_{x=0}(T)$$

whenever M is a diffeomorphism with $M(0) = 0$ and $dM_{x=0} =$ identity map and T is a distribution of compact support.
(c) Prove that if $g \in C_0^\infty(\mathbb{R}^n)$, then

$$\widehat{g(T \circ M)}(\ell) = (2\pi)^{-n} \iint g(x)\hat{T}(k) \exp[i(k \cdot M(x) - \ell \cdot x)]\, dx\, dk$$

in the sense that the integral formula is correct if $(1 + k^2)^{n+1/2}\hat{T}(k)$ is bounded and for fixed ℓ, the map

$$T \mapsto \text{integral}$$

is continuous in the norm $\|T\|_m = \sup_k \|(1 + k^2)^{-m}\hat{T}(k)\|$ for each $m > 0$. (*Hint*: Use the integration by parts machine based on $|(dM_x^*)^{-1} \operatorname{grad}_x(k \cdot M(x))| = |k|$.)
(d) Suppose k_0 is a unit vector with $k_0 \notin WF_{x=0}(T)$. Show that under the conditions in (b) one can pick open cones C_0 and C_1 about k_0 and a neighborhood N of $x = 0$ so that: (i) For every m,

$$\sup_{k \in C_1} (1 + k^2)^m |\widehat{gT}(k)| < \infty$$

for any g with $\operatorname{supp} g \subset N$.

(ii) $\quad \sup\{\ell \cdot [dM_x^*(k)]] \mid \ell \in C_0, k \notin C_1, x \in N; |\ell| = |k| = 1\} = \alpha < 1$

(e) Prove that for any m,

$$\sup_\ell \left| (1 + \ell^2)^m \int_{k \in C_1} g(x)\hat{T}(k) \exp[i(k \cdot M(x) - \ell \cdot x)]\, dx\, dk \right|$$

is finite. (*Hint*: Use (i) of (d) and the integration by parts machine based on $\ell^2 \exp(-i\ell \cdot x) = -\Delta_x[\exp(-i\ell \cdot x)]$.)

(f) Let

$$F(k, \ell) = \int g(x) \exp[i(k \cdot M(x) - \ell \cdot x)]\, dx$$

Prove that for any $m > 0$

$$\sup\{(1 + \lambda^2)^m F(\lambda k_0, \lambda \ell_0) \mid k_0 \notin C_1, \ell_0 \in C_0, |k_0 + \ell_0| = 1\} < \infty$$

Hint: Use (ii) of (d) and the integration by parts machine based on

$$|dM_x^*(k) - \ell|^{-2}\{(dM_x^*(k) - \ell) \cdot \operatorname{grad}_x[k \cdot M(x) - \ell \cdot x]\} = 1$$

(g) Prove that $\sup_{k \notin C_1, \ell \in C_0} (1 + |k| + |\ell|)^m F(k, \ell) < \infty$ for all m and conclude that $k \notin WF_{x=0}(T \circ M)$.
(h) Use symmetry and the result $WF_{x=0}(T \circ M) \subset WF_{x=0}(T)$ just proven to conclude the proof.

†76. The purpose of this problem is to outline the proofs of Theorems IX.13 and IX.14.
(a) Prove that $e^{b|x|} f \in L^2$ for all $b < a$ if and only if $e^{\eta \cdot x} f \in L^2$ for all $\eta \in \mathbb{R}^n$ with $|\eta| < a$.
(b) If $e^{b|x|} f \in L^2$ for all $b < a$, prove that $\hat{f}(\cdot)$ has an analytic continuation to $\{z \| \operatorname{Im} z| < a\}$ and that $\hat{f}(\cdot + i\eta) = \widehat{e^{\eta \cdot x} f}$. Conclude that the bound in Theorem IX.13 holds.
(c) Suppose that $\hat{f}$ has an analytic continuation to the tube $\{z \| \operatorname{Im} z| < a\}$ with the given bound. Use the Cauchy integral theorem to prove that for any $g \in C_0^\infty(\mathbb{R}^n)$ and $\eta \in \mathbb{R}^n$ with $|\eta| < a$,

$$\int \overline{g(x)} f(x)\, dx = \int \overline{\hat{g}(k - i\eta)} \hat{f}(k + i\eta)\, dk$$

(d) Prove that if f obeys the hypotheses of (c) and if $h_\eta = \hat{f}(\cdot + i\eta)$, then $\widehat{h_\eta(x)} = e^{\eta \cdot x} f$ almost everywhere and so conclude the proof of Theorem IX.13.
(e) By mimicking the above, prove Theorem IX.14.

77. (a) Use Hunt's interpolation theorem to prove that if $p^{-1} + q^{-1} = r^{-1}$, p and q less than ∞, $r > 1$, and if $f \in L^p(\mathbb{R}^n)$, $g \in L^q_w(\mathbb{R}^n)$, then $fg \in L^r_w(\mathbb{R}^n)$.
(b) Show that *if* the Marcinkiewicz interpolation theorem held without the restriction $p_i \le q_i$, then it would follow that $f \in L^4(\mathbb{R}^n)$ and $g \in L^4_w(\mathbb{R}^n)$ implies that $fg \in L^2(\mathbb{R}^n)$.
(c) Find explicit functions $f \in L^4(\mathbb{R}^n)$ and $g \in L^4_w(\mathbb{R}^n)$ so that $fg \notin L^2(\mathbb{R}^n)$.

78. (the uncertainty principle) Let $P = -i\hbar(d/dx)$ and $Q = x$ be operators on $L^2(\mathbb{R})$. Let $\varphi \in \mathscr{S}(\mathbb{R})$ with $\|\varphi\| = 1$ and define:

$$m_p = (P\varphi, \varphi), \qquad m_q = (Q\varphi, \varphi)$$
$$\sigma_p^2 = \|(P - m_p)\varphi\|^2, \qquad \sigma_q^2 = \|(Q - m_q)\varphi\|^2$$

(a) Using the commutation relation $PQ - QP = -i\hbar$, prove that $\sigma_p \sigma_q \ge \hbar/2$.
(b) Restate the result of part (a) in terms of μ_q and μ_p, the spectral measures of φ for Q and for P, and explain what this means for measurements of position and momentum in quantum mechanics (see Section VIII.11).
(c) Reformulate the result of part (a) as a statement about the Fourier transform.

READER'S GUIDE

Chapter IX is essentially self-contained and the prerequisites for it are minimal. The reader should know the properties of the Lebesgue integral, the elementary notions of Hilbert and Banach spaces, and the definition and basic properties of the Schwartz space of rapidly decreasing functions and its dual, the tempered distributions. This material is covered in Chapters I–III and Sections V.1–V.3 of Volume I and in many other functional analysis texts. The occasional reference to theorems in Volume I is usually descriptive so that the reader familiar with another elementary text can understand the reference.

We give a section by section description below. Here is a summary: The most basic material in Chapter IX is in Sections 1, 2, and the first part of 3. The reader mainly interested in quantum mechanics should consult especially Sections 1, 2, the first part of 3, 4, 7, and have some acquaintance with Section 9 and the Appendix to Section 4. The reader interested in quantum field theory should consult Sections 1, 2, 3, and 8. For partial differential equations, he should consult Sections 1, 2, the first part of 3, 4, 5, 6, and 10.

The fundamental properties of the Fourier transform are presented in Sections 1, 2, 4, and the first part of 3. In Section 1, the Fourier transform is defined on $\mathscr{S}(\mathbb{R}^n)$ and extended to $\mathscr{S}'(\mathbb{R}^n)$ by the adjoint map. The Fourier inversion theorem is proven, and we define and investigate the properties of convolution. In Section 2 we study the range of the Fourier transform on the classical spaces, proving the Plancherel, Hausdorff–Young, and Bochner theorems. In the first part of Section 3 we prove the Paley–Wiener theorems characterizing the Fourier transforms of C^∞ functions and distributions with compact support. In the second part of Section 3 we prove a more difficult theorem characterizing the Fourier transforms of tempered distributions in $\mathbb{R}^4$ with supports in cones. The reader should skip this part on first reading unless he is interested in the Wightman axioms (Section 8). Finally, in Section 4 we present various L^p-estimates relating Fourier transforms and convolutions. The reader should know how to use the interpolation theorems given in the Appendix since they are the basic tool for proving the estimates. The idea of interpolation is beautiful, but the proofs of the interpolation theorems are involved, so the proofs in the Appendix should be skipped on first reading.

The remaining sections, 5–10, deal with more advanced material and applications. Sections 5 and 6 present applications of the Fourier transform to partial differential equations. In Section 5 we prove the existence of fundamental solutions for constant coefficient partial differential equations. In Section 6 we investigate the Sobolev spaces and prove that every weak solution of $\Delta u = f$ is in fact a strict solution (Weyl's lemma).

In Section 7, we use the Fourier transform to derive properties of the free quantum-mechanical Hamiltonian $H_0 = -\Delta$, its resolvent $(H_0 + \kappa^2)^{-1}$, and the group it generates $e^{-iH_0 t}$.

In Section 8, we present and discuss the Gårding–Wightman axioms for a Hermitian scalar quantum field theory. No previous acquaintance with quantum field theory is necessary for reading this section. We show how the Fourier transform may be used to determine the analytic continuation properties of the Wightman function and to prove the PCT theorem. The technical appendix is devoted to proving a representation formula for polynomially bounded, Lorentz invariant measures with support in the closed forward light cone.

In Section 9, we consider the question of which L^2 functions on $\mathbb{R}^n$ have a natural restriction to a lower dimensional submanifold. This material will not be applied until we investigate the spectrum of quantum mechanical Hamiltonians in Chapter XIII. On first

reading, the statement of Theorem IX.41 and the general idea of its proof should be understood, but the gory details should be omitted.

Section 10 is intended as an introduction to wave front sets and oscillatory integrals, two important tools for the study of partial differential equations with nonconstant coefficients. This theory can be used to give conditions on two distributions so that their product is well defined. The material in Section 10 is not used again in Volumes II and III.

X: Self-Adjointness and the Existence of Dynamics

People used to think that when a thing changes, it must be in a state of change and that when a thing moves, it is in a state of motion. This is now known to be a mistake. *B. Russell*

X.1 Extensions of symmetric operators

We begin this chapter by studying symmetric operators and their extensions. Primarily, we wish to answer two questions: When do symmetric operators have self-adjoint extensions and, if they do, how can the extensions be characterized? These questions are answered by von Neumann's theory of deficiency indices which we will develop using many of the techniques we have already used in proving the basic criterion for self-adjointness (Theorem VIII.3) in Chapter VIII.

It is useful to begin by explaining why symmetric, non-self-adjoint operators are of interest in the first place. Typically, in quantum mechanics or quantum field theory, physical reasoning gives a formal expression for the Hamiltonian of the system; it is usually a partial differential operator on an appropriate L^2 space. We say "formal" when the domain of the Hamiltonian is not specified. It is usually easy to find a dense domain on which the formal Hamiltonian is a well-defined and symmetric operator H. The quantum dynamics should be given by a unitary group, and we know from Stone's theorem (Theorem VIII.8) that the infinitesimal generator of such a group must be self-adjoint. If $\overline{H}$, the closure of H, is self-adjoint,

then we can use H. But if H is not self-adjoint, then we must ask: Does H have self-adjoint extensions? And if it has several, which one shall we choose to generate the dynamics? In the case where there are several self-adjoint extensions, they are usually distinguished by the *physics* of the system being described. The problem of choosing the "right" self-adjoint extension is not just a mathematical "technicality" but is intimately related to the physics. For further discussion, see Examples 1 and 2 in this section.

We remark that throughout this section we discuss the extensions of *closed* symmetric operators. There is no loss of generality since every symmetric operator has a closure, and the operator and its closure have the same closed extensions.

Theorem X.1 Let A be a closed symmetric operator on a Hilbert space $\mathscr{H}$. Then

(1a) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open upper half-plane.
(1b) $\dim[\mathrm{Ker}(\lambda I - A^*)]$ is constant throughout the open lower half-plane.
(2) The spectrum of A is *one* of the following:
  (a) The closed upper half-plane
  or (b) the closed lower half-plane
  or (c) the entire plane
  or (d) a subset of the real axis
(3) A is self-adjoint if and only if case (2d) holds.
(4) A is self-adjoint if and only if the dimensions in both (1a) *and* (1b) are zero.

Proof Let $\lambda = \nu + i\mu$, $\mu \neq 0$. Since A is symmetric,

$$\|(\lambda - A)\varphi\|^2 \geq \mu^2 \|\varphi\|^2 \tag{X.1}$$

for all $\varphi \in D(A)$. From this inequality and the fact that A is closed, it follows immediately that $\mathrm{Ran}(\lambda - A)$ is a closed subspace of $\mathscr{H}$. Furthermore,

$$\mathrm{Ker}(\lambda - A^*) = \mathrm{Ran}(\bar{\lambda} - A)^{\perp} \tag{X.2}$$

The proof of these statements are the same as the case $\lambda = i$ which is given in the proof of Theorem VIII.3.

We will show that if $\eta \in \mathbb{C}$ is small enough, $\mathrm{Ker}(\lambda - A^*)$ and $\mathrm{Ker}((\lambda + \eta) - A^*)$ have the same dimension. Let u in $D(A^*)$ lie in $\mathrm{Ker}((\lambda + \eta) - A^*)$ with $\|u\| = 1$. Suppose $(u, v) = 0$ for all $v \in \mathrm{Ker}(\lambda - A^*)$.

Then by (X.2) $u \in \mathrm{Ran}(\bar{\lambda} - A)$, so there is a $\varphi \in D(A)$ with $(\bar{\lambda} - A)\varphi = u$. Thus,

$$\begin{aligned} 0 = (((\lambda + \eta) - A^*)u, \varphi) &= (u, (\bar{\lambda} - A)\varphi) + \bar{\eta}(u, \varphi) \\ &= \|u\|^2 + \bar{\eta}(u, \varphi) \end{aligned}$$

This is a contradiction if $|\eta| < |\mu|$ since by (X.1) $\|\varphi\| \leq \|u\|/|\mu|$. Thus for $|\eta| < |\mu|$, there is no $u \in \mathrm{Ker}((\lambda + \eta) - A^*)$ which is in $\mathrm{Ker}(\lambda - A^*)^{\perp}$. A short argument with projections (Problem 4) now shows that

$$\dim[\mathrm{Ker}((\lambda + \eta) - A^*)] \leq \dim[\mathrm{Ker}(\lambda - A^*)]$$

The same argument shows that if $|\eta| < |\mu|/2$, then $\dim[\mathrm{Ker}(\lambda - A^*)] \leq \dim[\mathrm{Ker}((\lambda + \eta) - A^*)]$, so we conclude that

$$\dim[\mathrm{Ker}(\lambda - A^*)] = \dim[\mathrm{Ker}((\lambda + \eta) - A^*)] \qquad \text{if} \quad |\eta| < |\mu|/2$$

Since $\dim[\mathrm{Ker}(\lambda - A^*)]$ is locally constant, it equals a constant in the upper half-plane and equals a (possibly different) constant in the lower half-plane. This proves (1).

It follows from (X.1) that if $\mathrm{Im}\ \lambda \neq 0$, $\lambda - A$ always has a bounded left inverse and from (X.2) that the inverse is everywhere defined if and only if $\dim[\mathrm{Ker}(\bar{\lambda} - A^*)] = 0$. Thus it follows from part (1) that each of the open upper and lower half-planes is either entirely in the spectrum of A or entirely in the resolvent set. This, plus the fact that $\sigma(A)$ is closed proves (2). (3) and (4) are restatements of Theorem VIII.3. ∎

Corollary If A is a closed symmetric operator that is semibounded, i.e. $(A\varphi, \varphi) \geq -M\|\varphi\|^2$, then $\dim[\mathrm{Ker}(\lambda - A^*)]$ is constant for

$$\lambda \in \mathbb{C} \backslash [-M, \infty)$$

Proof This corollary follows from the proof of Theorem X.1. The same argument about the invariance of dimension can be carried out for real λ in $(-\infty, -M)$, thus connecting the upper and lower half-planes.

Corollary If a closed symmetric operator has at least one real number in its resolvent set, then it is self-adjoint.

Proof Since the resolvent set is open and contains a point on the real axis, it must contain points in both the upper and lower half-planes. The corollary now follows from part (3) of Theorem X.1.

Since the dimensions of the kernels of $i - A^*$ and $i + A^*$ play an important role, it is convenient to give them names.

Definition Suppose that A is a symmetric operator. Let

$$\mathscr{K}_+ = \mathrm{Ker}(i - A^*) = \mathrm{Ran}(i + A)^\perp$$
$$\mathscr{K}_- = \mathrm{Ker}(i + A^*) = \mathrm{Ran}(-i + A)^\perp$$

$\mathscr{K}_+$ and $\mathscr{K}_-$ are called the **deficiency subspaces** of A. The pair of numbers n_+, n_-, given by $n_+(A) = \dim[\mathscr{K}_+]$, $n_-(A) = \dim[\mathscr{K}_-]$ are called the **deficiency indices** of A.

We remark that it is possible for the deficiency indices to be any pair of nonnegative integers; and further it is possible for n_+ or n_- (or both) to equal infinity. The reader is asked to construct examples in Problem 1.

We now set about the task of constructing the closed symmetric extensions of A. Let B be such an extension. Then for $\varphi \in D(B^*)$, we have $(\psi, B^*\varphi) = (B\psi, \varphi) = (A\psi, \varphi)$ for all $\psi \in D(A)$. Thus $\varphi \in D(A^*)$ and $B^*\varphi = A^*\varphi$ so

$$A \subseteq B \subseteq B^* \subseteq A^* \tag{X.3}$$

We introduce two new sesquilinear forms on $D(A^*)$:

$$(\varphi, \psi)_A = (\varphi, \psi) + (A^*\varphi, A^*\psi)$$
$$[\varphi, \psi]_A = (A^*\varphi, \psi) - (\varphi, A^*\psi)$$

A subspace of $D(A^*)$ such that $[\varphi, \psi]_A = 0$ for all φ and ψ in the subspace will be called **A-symmetric**. When we refer to subspaces of $D(A^*)$ as **A-closed** or **A-orthogonal** we mean in the inner product given by the graph inner product $(\cdot, \cdot)_A$.

Lemma Let A be a closed symmetric operator. Then

(a) The closed symmetric extensions of A are the restrictions of A^* to A-closed, A-symmetric subspaces of $D(A^*)$.

(b) $D(A)$, $\mathscr{K}_+$, and $\mathscr{K}_-$ are A-closed, mutually A-orthogonal subspaces of $D(A^*)$ and

$$D(A^*) = D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$$

(c) There is a one-to-one correspondence between A-closed, A-symmetric subspaces S of $D(A^*)$ which contain $D(A)$ and the A-closed, A-symmetric subspaces S_1 of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$ given by $S = D(A) \oplus_A S_1$.

Proof To prove (a), notice that (X.3) implies that every symmetric extension of A is contained in A^*. Further, the extension is closed if and only if its domain is A-closed and the extension is symmetric if and only if its domain is A-symmetric.

To prove (b), notice that $D(A)$ is A-closed since A is closed, and $\mathscr{K}_+$ and $\mathscr{K}_-$ are A-closed since they are already closed in the weaker topology given by the usual inner product. The fact that the three subspaces are orthogonal is a straightforward calculation which we omit. Suppose $\psi \in D(A^*)$ and $\psi \perp_A D(A) \oplus_A \mathscr{K}_+ \oplus_A \mathscr{K}_-$. For $\varphi \in D(A)$, we have $(\varphi, \psi) + (A^*\varphi, A^*\psi) = (\varphi, \psi)_A = 0$, so

$$(\varphi, \psi) = -(A\varphi, A^*\psi)$$

Thus, $A^*\psi \in D(A^*)$ and $A^*A^*\psi = -\psi$. Since

$$(A^* + i)(A^* - i)\psi = (A^*A^* + I)\psi = 0,$$

we conclude that $(A^* - i)\psi \in \mathscr{K}_-$. But if $\varphi \in \mathscr{K}_-$, then

$$\begin{aligned} i(\varphi, (A^* - i)\psi) &= (\varphi, \psi) + (A^*\varphi, A^*\psi) \\ &= (\varphi, \psi)_A = 0 \end{aligned}$$

since $\psi \perp_A \mathscr{K}_-$. Thus, we must have $(A^* - i)\psi = 0$, which implies that $\psi \in \mathscr{K}_+$. Since $\psi \perp_A \mathscr{K}_+$, we conclude that $\psi = 0$ which completes the proof of (b).

Let S_1 be an A-closed, A-symmetric subspace of $\mathscr{K}_- \oplus_A \mathscr{K}_-$. Suppose that $\varphi = \varphi_0 + \varphi_1$, $\psi = \psi_0 + \psi_1$ with φ_0, $\psi_0 \in D(A)$; φ_1, $\psi_1 \in S_1$. Then $[\varphi_0, \psi_0]_A = 0$ since A is symmetric and $[\varphi_1, \psi_1]_A = 0$ since S_1 is A-symmetric. Further,

$$\begin{aligned} [\varphi_0, \psi_1]_A &= (A^*\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= (A\varphi_0, \psi_1) - (\varphi_0, A^*\psi_1) \\ &= 0 \end{aligned}$$

since $\varphi_0 \in D(A)$ and $\psi_1 \in D(A^*)$. A similar proof shows that $[\varphi_1, \psi_0]_A = 0$. Thus,

$$[\varphi, \psi]_A = [\varphi_0, \psi_0]_A + [\varphi_1, \psi_0]_A + [\varphi_0, \psi_1]_A + [\varphi_1, \psi_1]_A = 0$$

so $S = D(A) \oplus_A S_1$ is an A-symmetric subspace. S is A-closed since $D(A)$ and S_1 are A-closed and A-orthogonal.

Conversely, let S be an A-closed, A-symmetric subspace of $D(A^*)$ containing $D(A)$. Let $S_1 = S \cap (\mathscr{K}_+ \oplus_A \mathscr{K}_-)$. Then S_1 is clearly A-closed and A-symmetric. Now suppose that $\varphi \in S$. Then φ can be uniquely expressed $\varphi = \varphi_0 + \varphi_1$ where $\varphi_0 \in D(A)$ and $\varphi_1 \in \mathscr{K}_+ \oplus_A \mathscr{K}_-$. Since $D(A) \subset S$, we have $\varphi_0 \in S$ which implies $\varphi_1 \in S$ also. Thus $\varphi_1 \in S_1$ so $S = D(A) \oplus_A S_1$. This proves (c). ∎

We are now ready to prove the main theorem of this section.

Theorem X.2 Let A be a closed symmetric operator. The closed symmetric extensions of A are in one-to-one correspondence with the set of partial isometries (in the usual inner product) of $\mathscr{K}_+$ into $\mathscr{K}_-$. If U is such an isometry with initial space $I(U) \subseteq \mathscr{K}_+$, then the corresponding closed symmetric extension A_U has domain

$$D(A_U) = \{\varphi + \varphi_+ + U\varphi_+ \,|\, \varphi \in D(A), \varphi_+ \in I(U)\}$$

and

$$A_U(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+$$

If $\dim I(U) < \infty$, the deficiency indices of A_U are

$$n_\pm(A_U) = n_\pm(A) - \dim[I(U)]$$

Proof Let A_1 be a closed symmetric extension of A. From the lemma we know that $D(A_1) = D(A) \oplus_A S_1$ where S_1 is an A-closed A-symmetric subspace of $\mathscr{K}_+ \oplus \mathscr{K}_-$. If $\varphi \in S_1$, it can be written uniquely as $\varphi = \varphi_+ + \varphi_-$. Since S_1 is A-symmetric

$$\begin{aligned} 0 &= (A^*\varphi, \varphi) - (\varphi, A^*\varphi) \\ &= 2i(\varphi_-, \varphi_-) - 2i(\varphi_+, \varphi_+) \end{aligned}$$

which implies that

$$\|\varphi_+\|^2 = \|\varphi_-\|^2 \tag{X.4}$$

Since S_1 is a subspace of $\mathscr{K}_+ \oplus_A \mathscr{K}_-$, (X.4) shows that $\varphi_+ \mapsto \varphi_-$ is a well-defined isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$. Call the corresponding partial isometry U. Then

$$D(A_1) = \{\varphi + \varphi_+ + U\varphi_+ \,|\, \varphi \in D(A), \varphi_+ \in I(U)\} \tag{X.5}$$

and

$$A_1(\varphi + \varphi_+ + U\varphi_+) = A^*(\varphi + \varphi_+ + U\varphi_+) = A\varphi + i\varphi_+ - iU\varphi_+ \tag{X.6}$$

Conversely, let U be an isometry from a subspace of $\mathscr{K}_+$ into $\mathscr{K}_-$ and define $D(A_1)$ and A_1 by (X.5) and (X.6). Then $D(A_1)$ is an A-closed, A-symmetric subspace of $D(A^*)$, so by the lemma, A_1 is a closed symmetric extension of A.

The statement about deficiency indices follows by looking at the ranges of $i + A_1$ and $i - A_1$ on $D(A_1)$. ∎

Corollary Let A be a closed symmetric operator with deficiency indices n_+ and n_-. Then,

(a) A is self-adjoint if and only if $n_+ = 0 = n_-$.
(b) A has self-adjoint extensions if and only if $n_+ = n_-$. There is a one–one correspondence between self-adjoint extension of A and unitary maps from $\mathscr{K}_+$ onto $\mathscr{K}_-$.
(c) If either $n_+ = 0 \neq n_-$ or $n_- = 0 \neq n_+$, then A has no nontrivial symmetric extensions (such operators are called **maximal symmetric**).

Example 1 We will consider the example introduced in Section VIII.2 from several points of view. Let T be the operator $i\,d/dx$ on $L^2(0, 1)$ with the domain $D(T) = \{\varphi \,|\, \varphi \in AC[0, 1], \varphi(0) = 0 = \varphi(1)\}$. We showed in Section VIII.2 that T^* is the operator $i\,d/dx$ with domain $D(T^*) = AC[0, 1]$.

Since the operator T is so simple and since we know the domain of its adjoint explicitly, we can determine the self-adjoint extensions of T without using the machinery developed in this section. It is instructive to do that first. Suppose S is a symmetric extension of T. Since $D(S^*) \subset D(T^*)$, we know that the functions in $D(S^*)$ are absolutely continuous and $S^*\varphi = i\,d\varphi/dx$. Thus for $\varphi \in D(S)$ and $\psi \in D(S^*)$, integration by parts shows that

$$(S\varphi, \psi) - (\varphi, S^*\psi) = \overline{\varphi(1)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0 \tag{X.7}$$

In the case $S = T$ we can see why T is not self-adjoint. The boundary conditions on the functions in $D(T)$ are so strong that no boundary conditions on the functions in $D(T^*)$ are necessary in order to ensure that the right-hand side of (X.7) equals zero. What is necessary is to extend the set of functions in $D(S)$ by allowing more general boundary conditions so that the equality (X.7) requires the *same* boundary conditions on the functions in $D(S^*)$. We now do this. Let S be a self-adjoint extension of T and suppose that $\varphi \in D(S)\backslash D(T)$. Then (X.7) requires that $|\varphi(1)|^2 = |\varphi(0)|^2$ and since $\varphi \notin D(T)$, $\varphi(0) \neq 0$, so there is an α with $|\alpha| = 1$ so that $\varphi(1) - \alpha\varphi(0) = 0$. If ψ is any other function in $D(S)$, then (X.7) requires that $\psi(1) = \alpha\psi(0)$ with the *same* α. Thus, $S \subset T_\alpha$ where $T_\alpha = i\,d/dx$ on

$$D(T_\alpha) = \{\varphi \,|\, \varphi \in AC[0, 1], \varphi(1) = \alpha\varphi(0)\}$$

Since T_α is symmetric and S is self-adjoint, $S = T_\alpha$ for some α.

Next, we determine which T_α are self-adjoint. Choose $\varphi \in D(T_\alpha)$ and $\psi \in D(T_\alpha^*)$. Then (X.7) requires that

$$\bar{\alpha}\,\overline{\varphi(0)}\psi(1) - \overline{\varphi(0)}\psi(0) = 0$$

so that $\psi(1) = \alpha\psi(0)$. Thus $\psi \in D(T_\alpha)$, so $D(T_\alpha^*) = D(T_\alpha)$, i.e. T_α is self-adjoint for each α. Thus, the set of self-adjoint extensions of T consists of the collection of operators $\{T_\alpha | \alpha \in \mathbb{C}, |\alpha| = 1\}$.

We now show how the machinery of this section leads to the same result. To determine $\mathscr{K}_+$, we must find the solutions of $T^*\psi = i\psi$. If $\psi \in D(T^*)$, then $\psi \in AC[0, 1]$, and the equality $i\, d\psi/dx = i\psi$ shows that ψ' is also absolutely continuous. Repeating this argument shows that any solution of $T^*\psi = i\psi$ is in fact infinitely differentiable and satisfies $\psi' = \psi$. Thus $\mathscr{K}_+ = \{ce^x | c \in \mathbb{C}\}$, and similarly $\mathscr{K}_- = \{ce^{-x} | c \in \mathbb{C}\}$. Therefore, the deficiency indices of T are $\langle 1, 1\rangle$. Let

$$\varphi_+ = \frac{\sqrt{2}}{\sqrt{e^2 - 1}} e^x \qquad \text{and} \qquad \varphi_- = \frac{\sqrt{2}\, e}{\sqrt{e^2 - 1}} e^{-x}$$

be normalized vectors from $\mathscr{K}_\pm$. Then the only partial isometries of $\mathscr{K}_+$ into $\mathscr{K}_-$ are the maps $\varphi_+ \mapsto \gamma\varphi_-$ where $|\gamma| = 1$. By Theorem X.2, the only symmetric extensions of T are the operators $A_\gamma = i\, d/dx$ with domain

$$D(A_\gamma) = \{\varphi + \beta\varphi_+ + \gamma\beta\varphi_- \,|\, \varphi \in D(T), \beta \in \mathbb{C}\}$$

By the last statement of Theorem X.2, each A_γ has zero deficiency indices and is therefore self-adjoint. To see that these are the same operators we got before, notice that if $\psi \in D(A_\gamma)$, then

$$\psi(0) = \frac{\beta(1 + \gamma e)\sqrt{2}}{\sqrt{e^2 - 1}} \qquad \text{and} \qquad \psi(1) = \frac{\sqrt{2}\,\beta(\gamma + e)}{\sqrt{e^2 - 1}}$$

so

$$\psi(1) = \frac{\gamma + e}{1 + \gamma e}\psi(0) = \alpha\psi(0) \qquad \text{where} \quad |\alpha| = \left|\frac{\gamma + e}{1 + \gamma e}\right| = 1$$

Conversely, if $\psi(1) = \alpha\psi(0)$, then ψ can be written $\psi = \varphi + \beta\varphi_+ + \gamma\beta\varphi_-$ for some β where $\gamma = (\alpha - e)/(1 - \alpha e)$. Thus, $A_\gamma = T_\alpha$.

We now examine the same problem from a "physical" point of view. Suppose that we have a smooth wave packet $\varphi(x)$ on $[0, 1]$ which is zero near the end points and which is being translated to the right (Figure X.1). For small enough y (so that the packet does not get to the end), the translations are given by the family of operators $U(y)$: $\varphi(x) \to \varphi(x - y)$. In quantum mechanics, translation should be represented by a unitary group whose generator is the momentum operator. For the wave packet $\varphi(x)$, this is the case:

$$\lim_{y \to 0} \frac{U(y)\varphi - \varphi}{iy} = \lim_{y \to 0} \frac{\varphi(x - y) - \varphi(x)}{iy} = i\frac{d}{dx}\varphi$$

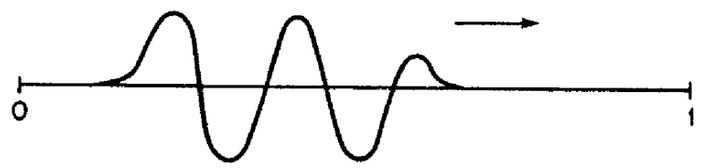


FIGURE X.1 The wave packet $\varphi(x)$.

So, the generator of translation acts like $i\, d/dx$ on the functions with support away from the end points. In fact, $i\, d/dx$ is symmetric on $C_0^1(0, 1)$, the C^1 functions of compact support on $(0, 1)$, and its closure is just our operator T. But T is not self-adjoint and the reason is clear: We have specified the translation $U(y)$ only for functions whose support does not contain zero or one and then only for sufficiently small y (depending on the support). We must specify what happens when the wave packet gets to the end! If we want translation to be represented by a unitary group, then what goes out at one end must come in at the other (as though the interval $[0, 1]$ were bent into a circle). That is, unitarity requires

$$\int_0^1 |\varphi(x - y)|^2\, dx = \int_0^1 |\varphi(x)|^2\, dx$$

where $x - y$ means translation mod 1. However, we still have the freedom of choosing the phase of the wave packet as it comes in at zero. By the superposition principle all functions must change by the same phase when they come back in. Thus the different "translations" are just given by specifying α, $|\alpha| = 1$ and by requiring that all reasonable wave packets $\psi_y \equiv \varphi(\cdot + y)$ satisfy $\psi_y(1) = \alpha\psi_y(0)$ for *all* times y. This motion is just given by e^{iyT_α} where T_α is the operator described above. Thus, even in this physically trivial situation we see that *different* self-adjoint extensions correspond to *different physics*.

A simple and useful criterion for a symmetric operator to have self-adjoint extensions is given by the following theorem.

Definition An antilinear map C: $\mathscr{H} \to \mathscr{H}$ $(C(\alpha\varphi + \beta\psi) = \bar{\alpha}C\varphi + \bar{\beta}C\psi)$ is called a **conjugation** if it is norm-preserving and $C^2 = I$.

Theorem X.3 (von Neumann's theorem) Let A be a symmetric operator and suppose that there exists a conjugation C with C: $D(A) \to D(A)$ and $AC = CA$. Then A has equal deficiency indices and therefore has self-adjoint extensions.

Proof Since $C^2 = I$ and $CD(A) \subseteq D(A)$, we have $CD(A) = D(A)$. Suppose that $\varphi_+ \in \mathscr{K}_+$ and $\psi \in D(A)$. Then

$$\begin{aligned} 0 &= \overline{(\varphi_+, (A + i)\psi)} = (C\varphi_+, C(A + i)\psi) \\ &= (C\varphi_+, (A - i)C\psi) \end{aligned}$$

Since C takes $D(A)$ onto $D(A)$, $C\varphi_+ \in \mathscr{K}_-$, so $C: \mathscr{K}_+ \to \mathscr{K}_-$. A similar proof shows that $C: \mathscr{K}_- \to \mathscr{K}_+$. Since C preserves norms,

$$\dim[\mathscr{K}_+] = \dim[\mathscr{K}_-] \quad \blacksquare$$

Example 2 (Schrödinger particle on a half-line) Let A be the operator $-d^2/dx^2$ on $L^2(0, \infty)$ with domain $C_0^\infty(0, \infty)$. Since complex conjugation commutes with A, we immediately know from Theorem X.3 that the deficiency indices of A are equal. We want to find the solutions of $A^*\varphi = \pm i\varphi$. Since $L^2(0, \infty) \subset \mathscr{D}'_{(0,\infty)}$, we are just looking for weak solutions (see Section V.4) of $-d^2\varphi/dx^2 = \pm i\varphi$. It follows from the regularity theorem (Theorem IX.25) that these solutions are infinitely differentiable and thus strong solutions. By elementary ordinary differential equations the strong solutions of $-\varphi''(x) = +i\varphi(x)$ are

$$\exp((-1 + i)x/\sqrt{2}), \qquad \exp((1 - i)x/\sqrt{2})$$

and the strong solutions of $-\varphi''(x) = -i\varphi(x)$ are $\exp((1 + i)x/\sqrt{2})$, $\exp((-1 - i)x/\sqrt{2})$. Since only $\exp((-1 + i)x/\sqrt{2})$ and $\exp((-1 - i)x/\sqrt{2})$ are in $L^2(0, \infty)$, we see that the deficiency indices are $\langle 1, 1\rangle$. Using Theorem X.2 and an analysis similar to the second part of Example 1, the reader can easily show (Problem 5) that the self-adjoint extensions of A can be parametrized by $\mathbb{R} \cup \{\infty\}$ with

$$D(A_a) = \{\psi \,|\, \psi \in AC^2[0, \infty], \psi'(0) + a\psi(0) = 0\}$$

if $a \in \mathbb{R}$ and

$$D(A_\infty) = \{\psi \,|\, \psi \in AC^2[0, \infty], \psi(0) = 0\}$$

The extensions all act on their respective domains by $-d^2/dx^2$. $AC^2[0, 1]$ is just the set of functions in $L^2[0, 1]$ whose weak derivatives are in $AC[0, 1]$, in particular, they are continuously differentiable.

The physical interpretation of these boundary conditions is as follows. Since the momentum operator is $i^{-1}\, d/dx$ and $i^{-1}\,(d/dx)e^{-ikx} = -ke^{-ikx}$, the function e^{-ikx} is a plane wave moving to the left with momentum

$k > 0$, i.e. an incoming wave of momentum k. e^{ikx} is an outgoing wave of momentum k. Let $a < \infty$ be fixed. The functions e^{ikx} and e^{-ikx} are not in $L^2(0, \infty)$ because of their behavior at ∞, but we ignore that since we are interested in behavior around the origin. Neither e^{ikx} or e^{-ikx} is in $D(A_a)$ near zero since they do not satisfy the boundary conditions. But if $\alpha = (ik - a)/(ik + a)$, then $e^{-ikx} + \alpha e^{ikx}$ satisfies the boundary conditions $\psi'(0) + a\psi(0)$ and is in $D(A_a)$ (ignoring the behavior at ∞). Thus the operator A_a generates the dynamics in which a plane wave of momentum k is reflected at the origin with the change of phase $\alpha(k) = (ik - a)/(ik + a)$. The case $a = \infty$ corresponds to a hard wall potential where the phase change for all momenta is $\alpha = -1$. Notice that the phase change for various plane waves is different for the different self-adjoint extensions. Thus, the *different* self-adjoint extensions correspond to *different* physics.

A less trivial application of Theorem X.3 is used in the following example in which only the *existence* of some self-adjoint extension is needed. The reader should compare this example to the similar proof of Bochner's theorem (Theorem IX.9) where the corresponding existence statement was derived from Stone's theorem.

Example 3 (the Hamburger moment problem) Let ρ be a positive measure on $\mathbb{R}$ and define

$$a_n = \int_{-\infty}^{\infty} x^n \, d\rho(x) \tag{X.8}$$

The numbers a_n are called the **moments** of the measure ρ. The Hamburger moment problem is to determine conditions on a sequence of real number $\{a_n\}_{n=0}^\infty$, so that there exists a measure satisfying (X.8). There is a very elegant solution.

Theorem X.4 A sequence of real numbers $\{a_n\}$ are the moments of a positive measure on $\mathbb{R}$ if and only if for all N and all $\beta_0, \ldots, \beta_N \in \mathbb{C}$,

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} \geq 0 \tag{X.9}$$

Proof Suppose first that ρ is a positive measure and (X.8) holds. Then

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} = \int_{-\infty}^{\infty} \left| \sum_{n=0}^{N} \beta_n x^n \right|^2 d\rho \geq 0$$

Conversely, suppose that (X.9) holds. Let P denote the set of polynomials on $\mathbb{R}$ with complex coefficients and define a sesquilinear form on P by

$$\left(\sum_{n=0}^{N}\beta_n x^n,\ \sum_{m=0}^{M}\alpha_m x^m\right)=\sum_{n=0}^{N}\sum_{m=0}^{M}\bar{\beta}_n\alpha_m a_{n+m}$$

By (X.9) the form is nonnegative. Let $Q=\{\psi\,|\,\psi\in P,(\psi,\psi)=0\}$ and let $\mathscr{H}$ be the Hilbert space obtained by completing P/Q in the inner product $(\cdot,\cdot)$. Consider the map $A\colon P\to P$ defined by

$$A\colon \sum_{n=0}^{N}\beta_n x^n\to\sum_{n=0}^{N}\beta_n x^{n+1}$$

It is not hard to see that A is symmetric and $A\colon Q\to Q$ since the Schwarz inequality implies that

$$(A\psi,A\psi)=|(A^2\psi,\psi)|\le(A^2\psi,A^2\psi)^{1/2}(\psi,\psi)^{1/2}$$

Thus, A lifts to a symmetric operator $\hat{A}$ on $\mathscr{H}$ with domain P/Q. If C denotes the usual complex conjugation on P, then C also lifts to a map $\hat{C}\colon P/Q\to P/Q$. It is easily checked that $\hat{C}$ extends to a conjugation on $\mathscr{H}$ and $\hat{A}\hat{C}=\hat{C}\hat{A}$. By Theorem X.3, $\hat{A}$ has some self-adjoint extension, call it $\tilde{A}$. Let ρ be the spectral measure for the vector 1 in P. Then

$$\int x^n\,d\rho(x)=(1,\tilde{A}^n1)=(1,x^n)=a_n\ \blacksquare$$

In Chapter XVI we will see that the Hahn–Banach theorem can be used to provide another proof of Theorem X.4. In Section X.6, we discuss the uniqueness aspects of the Hamburger moment problem.

Appendix to X.1 Motion on a half-line, limit point–limit circle methods

Any blockhead can cite generalities, but the mastermind discerns the particular cases they represent. — *George Eliot in* ***Daniel Deronda***

In this appendix, we discuss both the classical motion and the quantum-mechanical motion of a particle in a potential on a half-line. Comparing these two cases brings out nicely both the analogies and the differences between classical and quantum mechanics and provides an opportunity to apply the theorems on deficiency indices to derive the limit point–limit circle theory of ordinary differential equations. Furthermore, information about quantum-mechanical problems on a half-line can be used to analyze spherically symmetric multidimensional problems (see Example 4).

We begin with the classical case. Let $x(t)$ and $v(t)$ be the position and velocity of a particle moving on the half-line $(0,\infty)$ in a potential $V(x)$ which we assume has a continuous derivative $V'(x)$ which is Lipschitz uniformly on every compact subset of $(0,\infty)$. The Hamiltonian for the system is $H(x,v)=\frac{1}{2}mv^2+V(x)$ and the equations of motion are

$$\dot{x}(t)=v(t),\qquad \dot{v}(t)=\frac{-1}{m}V'(x(t)) \tag{X.10}$$

For each given $x_0>0$, v_0, $t_0>0$, the standard contraction mapping argument (see Section V.6) gives the existence of a unique solution pair $\langle x(t),v(t)\rangle$ for t near t_0 satisfying $x(t_0)=x_0$, $v(t_0)=v_0$. The following proposition shows that the only case where a local solution does not extend to a global solution is when the particle runs into zero or off to infinity in finite time.

Proposition 1 Suppose that a global solution of (X.10) satisfying $x(t_0)=x_0>0$, $v(t_0)=v_0$ does not exist, that is, the maximal interval on which the solution with the initial conditions exists is $[t_0,\tau)$ where $\tau<\infty$. Then either

$$\lim_{t\uparrow\tau}x(t)=0\qquad\text{or}\qquad\lim_{t\uparrow\tau}x(t)=\infty$$

Proof By the construction of local solutions in Section V.6, and the assumptions made above on $V(x)$, for any compact subset K of $(0,\infty)\times\mathbb{R}$, there is a T_K so that (X.10) has a unique solution for $t\in(t_1-T_K,t_1+T_K)$ with specified values $\langle x_1,v_1\rangle\in K$ at $t=t_1$. From this we see that if the solution cannot be extended past $t=\tau$, then it cannot lie in K for any $t>\tau-T_K$. To complete the proof we must strengthen this statement that the point $\langle x(t),v(t)\rangle$ must eventually leave any compact subset of the phase space $(0,\infty)\times\mathbb{R}$ to the statement that $x(t)$ eventually leaves any compact subset C of $(0,\infty)$. It is here that conservation of energy enters critically. Since $H(x(t),v(t))=H(x_0,v_0)=E_0$, if $x(t)$ lies in some compact subset C, then $\langle x(t),v(t)\rangle$ is contained in the compact set

$$C\times\left\{v(t)\,\middle|\,|v(t)|\le\sqrt{\frac{2}{m}}\left(E_0-\inf_{x\in C}V(x)\right)^{1/2}\right\}$$

Thus for each n there is a t_n so that $x(t)\notin(1/n,n)$ for $t>t_n$ which by the continuity of $x(t)$ proves the proposition. $\blacksquare$

The above argument shows how conservation of energy may be used to prove global existence for a classical system of one degree of freedom. In Section X.13 we will use the same energy conservation method to prove global existence for a classical system with an infinite number of degrees of freedom.

Definition We say that the classical motion generated by V is **complete** at 0 (respectively at ∞) if there is no $\langle x_0, v_0\rangle \in (0, \infty) \times \mathbb{R}$ so that the solution $x(t)$ runs off to 0 (respectively to ∞) in a finite time.

Thus if V is complete at both 0 and ∞, global solutions exist for all initial conditions $\langle x_0, v_0\rangle$. The following theorem settles the question of when V is complete.

Theorem X.5 Let $V(x)$ have a continuous derivative which is uniformly Lipschitz on each compact subset of $(0, \infty)$. Then the classical motion generated by $V(x)$:

(a) is not complete at 0 if and only if $V(x)$ is bounded above near zero;
(b) is not complete at ∞ if and only if V is bounded above for $x \geq 1$ and

$$\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty \qquad \text{for some } K > \sup_{x \geq 1} V(x)$$

Proof V is not bounded above at zero if and only if there is a sequence $x_n \to 0$ so that $V(x_n) \to \infty$. Suppose V is not bounded above at zero. By conservation of energy

$$\tfrac{1}{2}mv(t)^2 + V(x(t)) = \tfrac{1}{2}mv_0^2 + V(x_0)$$

so $V(x(t)) \leq \frac{1}{2}mv_0^2 + V(x_0)$. Thus $x(t)$ can never equal x_n for n sufficiently large and so $x(t)$ can never get near zero. Thus V is complete at zero. Conversely, suppose $V(x) \leq M$ on $(0, 1)$. Let $x(0) = x_0 = 1$ and choose v_0 negative and so that $\frac{1}{2}mv_0^2 + V(1) = 1 + M$. Then $\frac{1}{2}mv(t)^2 \geq 1$ for all t so the particle gets to zero in a finite time. This proves (a).

If $V(x)$ is not bounded above on $(1, \infty)$, then the same argument as above shows that V is complete at ∞. So, suppose that $V(x) \leq M$ for $x \in [1, \infty)$, and that for some initial conditions $\langle x_0, v_0\rangle$ and a $\tau < \infty$, $\tau \in \mathbb{R}$ we have $\lim_{t \to \tau} x(t) = \infty$. Let $K = \max\{M + 1, \frac{1}{2}mv_0^2 + V(x_0)\}$. Then, for all $t \in (0, \tau)$,

$$\left|\frac{dx}{dt}\right| \leq \sqrt{\frac{2}{m}}\sqrt{K - V(x(t))}$$

Once the motion starts going to the right, $x(t)$ must be strictly increasing because if it were not, conservation of energy and the uniqueness of solutions of (X.10) imply that it would never get to ∞. Thus there is a $t_1 < \tau$ so that $t \in (t_1, \tau)$ implies $dx/dt > 0$ and $x(t) \geq 1$. Therefore

$$\sqrt{\frac{m}{2}}\int_{x(t_1)}^\infty \frac{dx}{\sqrt{K - V(x)}} \leq \int_{x(t_1)}^\infty \frac{dt}{dx}\,dx = \tau - t_1 < \infty$$

Conversely, if

$$\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty \qquad \text{for some } K > \sup_{x \geq 1} V(x)$$

we choose initial conditions $x_0 = 1$, $v_0 > 0$, so that $E = \frac{1}{2}mv_0^2 + V(x_0) = K$. Then $dx/dt > 0$ for all $t > 0$ and

$$\int_0^\infty \left(\frac{dt}{dx}\right) dx = \sqrt{\frac{m}{2}}\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} < \infty$$

so the travel time to ∞ is finite. ∎

We turn now to the quantum-mechanical case where we need only assume that $V(x)$ is a real-valued, continuous function on $(0, \infty)$. The quantum analogue of the classical Hamiltonian $H(x, v)$ is the formal operator $-(2m)^{-1}\,d^2/dx^2 + V(x)$. We will denote by H the operator $-d^2/dx^2 + V(x)$ on $L^2(0, \infty)$ with domain $D(H) = C_0^\infty(0, \infty)$, the C^∞ functions with support away from 0 and ∞ (we drop the inessential $1/2m$). Using the fact that $V(x)$ is real-valued and a simple integration by parts, we see that H is a symmetric operator. Suppose that $\psi \in D(H^*)$, then

$$\left(-\frac{d^2}{dx^2}\varphi + V\varphi, \psi\right) = (\varphi, H^*\psi)$$

or

$$\left(-\frac{d^2}{dx^2}\varphi, \psi\right) = (\varphi, H^*\psi) - (\varphi, V\psi)$$

for all $\varphi \in C_0^\infty(0, \infty)$. Thus the second weak derivative of ψ is locally L^2 since $V(x)\psi(x)$ is locally L^2. By Sobolev's lemma, ψ' is absolutely continuous and $-\psi'' - V\psi \in L^2(0, \infty)$ (although each of the separate terms may not be in L^2 near zero or infinity). Therefore, the functions in $D(H^*)$ are quite nice and the action of H^* is just what we expect. Finally, we note that H commutes with complex conjugation so its deficiency indices are equal. We summarize in a proposition.

Proposition 2 Suppose $V(x)$ is a real valued continuous function on $(0, \infty)$ and let H be the operator $-d^2/dx^2 + V(x)$ with domain $C_0^\infty(0, \infty)$. Then

(a) H is symmetric.
(b) If $\psi \in D(H^*)$, then ψ is continuously differentiable, ψ' is absolutely continuous, ψ'' is locally L^2, $-\psi'' + V\psi \in L^2(0, \infty)$, and

$$H^*\psi = -\psi'' + V\psi$$

(c) H has equal deficiency indices.

The importance of Proposition 2 is that it shows that questions about the deficiency indices of H reduce to questions about the classical ordinary differential equations $-\psi'' + V\psi = \pm i\psi$. We prepare for our analysis with:

Proposition 3 Let $Q(x)$ be a continuous complex-valued function on $(0, \infty)$. Then the set of solutions of $\varphi''(x) = Q(x)\varphi(x)$ on $(0, \infty)$ is a two-dimensional vector space of twice continuously differentiable functions. For any two solutions φ and ψ, the **Wronskian** $W(x) = \varphi'(x)\psi(x) - \varphi(x)\psi'(x)$ is constant and equals zero if and only if φ and ψ are linearly dependent as functions.

Proof We will prove the existence of a global solution with arbitrarily specified data $\langle \varphi(1), \varphi'(1) \rangle \in \mathbb{C}^2$ at $x = 1$. By the discussion in Section V.6, local solutions exist, so as in the proof of Proposition 1, a global solution can fail to exist only if $\alpha(x) = \langle \varphi(x), \varphi'(x) \rangle$ goes to infinity at some finite x_0 different from zero. We will show that this cannot happen for any $x_0 > 1$; the proof for $x_0 < 1$ is similar. Define

$$q(x_0) = \sup\{|Q(x)| + 1 \mid 1 \le x \le x_0\}$$

Then, from the differential equation we have

$$\alpha'(x) = \langle \varphi'(x), Q(x)\varphi(x) \rangle$$

for $1 \le x \le x_0$, so

$$|\alpha'(x)| \le q(x_0)|\alpha(x)|$$

and

$$|\alpha(x)| \le |\alpha(1)| + q(x_0)\int_1^x |\alpha(y)|\, dy \qquad \text{(X.11)}$$

Thus, by iterating (X.11),

$$|\alpha(x)| \le |\alpha(1)| e^{q(x_0)(x-1)}$$

for $1 \le x \le x_0$. This proves the existence of at least two independent global solutions. Furthermore, by local uniqueness there are at most two, so there are exactly two.

The statements about $W(x)$ follow immediately by differentiation and by observing that $W(x)$ is the determinant of

$$\begin{pmatrix} \psi & \varphi \\ \psi' & \varphi' \end{pmatrix} \blacksquare$$

We now investigate the deficiency indices of H by studying the solutions of

$$-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x) \qquad \text{(X.12)}$$

Theorem X.6 Let $V(x)$ be a continuous real-valued function on $(0, \infty)$.

(a) If $\operatorname{Im} \lambda \neq 0$, then at least one nonzero solution of (X.12) is in L^2 near zero and at least one solution is in L^2 near ∞.
(b) If for one $\lambda \in \mathbb{C}$, both solutions of (X.12) are in L^2 near infinity (respectively near zero) then, for *all* $\lambda \in \mathbb{C}$, both solutions of (X.12) are in L^2 near infinity (respectively near zero).

Proof Consider first the operator B on $L^2(1, 2)$ with domain $D(B) = \{u \in AC^2[1, 2] \mid u(1) = u(2) = u'(1) = u'(2) = 0\}$ and with $Bu = -u'' + Vu$. By mimicking the arguments used in Examples 1 and 2 of Section X.1 and by using Proposition 3, one finds that B has deficiency indices $\langle 2, 2 \rangle$. In particular, if $\operatorname{Im} \lambda \neq 0$, $\operatorname{Ran}(B - \lambda)$ is not dense in $L^2(1, 2)$. We can thus find $v \in C_0^\infty(1, 2)$ with $v \notin \operatorname{Ran}(B - \lambda)$.

Now, let $\tilde{H}$ be a self-adjoint extension of the operator H on $L^2(0, \infty)$. Since $\operatorname{Im} \lambda \neq 0$, we can find $u \in D(\tilde{H}) \subset D(H^*)$ satisfying $(\tilde{H} - \lambda)u = v$. It is impossible that u vanish identically on both $(0, 1)$ and $(2, \infty)$, for if it did, its restriction to $[1, 2]$ would lie in $D(B)$ thereby contradicting the condition that $v \notin \operatorname{Ran}(B - \lambda)$.

Suppose that u does not vanish identically on $(0, 1)$. Then the restriction $\tilde{u}$ of u to $(0, 1)$ satisfies (X.12) on $(0, 1)$ and is square integrable near 0. Let $D(A) = \{f \in D(\tilde{H}) \mid f \equiv 0 \text{ in } [1, \infty)\}$, viewed as a (dense) subset of $L^2(0, 1)$. The operator $A - \lambda \equiv (\tilde{H} - \lambda) \restriction D(A)$ does not have dense range since $\bar{\tilde{u}}$, the complex conjugate of $\tilde{u}$, obeys: $\bar{\tilde{u}} \in D(A^*)$ and $(A^* - \bar{\lambda})\bar{\tilde{u}} = 0$. As a result, we can find $w \in C_0^\infty(0, 1)$ with $w \notin \operatorname{Ran}(A - \lambda)$. Since $\tilde{H}$ is self-adjoint, we can find $f \in D(\tilde{H})$ with $(\tilde{H} - \lambda)f = w$. Since $w \notin \operatorname{Ran}(A - \lambda)$,

f cannot vanish identically in $[1, \infty)$ and we thereby obtain a nonzero solution of (X.12) square integrable near ∞. If u does not vanish identically on $(2, \infty)$, a similar argument can be used. This proves (a).

To prove (b), let us suppose that φ_1 and φ_2 are two independent solutions of (X.12) for some $\lambda_0 \in \mathbb{C}$ and that both φ_1 and φ_2 are L^2 near ∞, and are normalized so that $\varphi_1'(x)\varphi_2(x) - \varphi_1(x)\varphi_2'(x) = 1$. Let u be a solution of (X.12) for $\lambda = \lambda_1 \neq \lambda_0$. Choose $c \in (0, \infty)$. Then an explicit computation shows that

$$u(x) - (\lambda_1 - \lambda_0)\int_c^x (\varphi_1(x)\varphi_2(\xi) - \varphi_1(\xi)\varphi_2(x))u(\xi)\, d\xi$$

satisfies (X.12) with $\lambda = \lambda_0$, so

$$u(x) = c_1\varphi_1(x) + c_2\varphi_2(x) + (\lambda_1 - \lambda_0)\int_c^x (\varphi_1(x)\varphi_2(\xi) - \varphi_1(\xi)\varphi_2(x))u(\xi)\, d\xi$$

for some constants c_1 and c_2. Define $\|f\|^2_{[c,x]} = \int_c^x |f(x)|^2\, dx$ and choose M so that $\|\varphi_1\|_{[c,\infty]} < M$ and $\|\varphi_2\|_{[c,\infty]} < M$. Then, by the Schwarz inequality,

$$|u(x)| \leq |c_1||\varphi_1(x)| + |c_2||\varphi_2(x)| + |\lambda_1 - \lambda_0|(|\varphi_1(x)| + |\varphi_2(x)|)M\|u\|_{[c,x]}$$

so

$$\|u\|_{[c,x]} \leq |c_1|M + |c_2|M + 2M^2|\lambda_1 - \lambda_0|\|u\|_{[c,x]}$$

Thus if $|\lambda_1 - \lambda_0| \leq 1/4M^2$, $\frac{1}{2}\|u\|_{[c,x]} \leq (|c_1| + |c_2|)M$ for all x, so u is in L^2 near ∞. Since we can choose M as small as we like by choosing c large, we have proven (b) for the case at infinity. The case at zero is proved similarly. ∎

We will say that $V(x)$ is in the **limit circle case** at infinity (respectively at zero) if for some, and therefore all, λ, *all* solutions of

$$-\varphi''(x) + V(x)\varphi(x) = \lambda\varphi(x)$$

are square integrable at infinity (respectively at zero). If $V(x)$ is not in the limit circle case at infinity (respectively at zero), it is said to be in the **limit point case**. For the origin of this terminology, see the Notes. We can now prove:

Theorem X.7 (Weyl's limit point–limit circle criterion) Let $V(x)$ be a continuous real-valued function $(0, \infty)$. Then $H = -d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(0, \infty)$ if and only if $V(x)$ is in the limit point case at both zero and infinity.

Proof If $V(x)$ is in the limit circle case at both zero and infinity, then the deficiency indices of H are $\langle 2, 2\rangle$. If $V(x)$ is limit circle at one end and limit point at the other, then H has deficiency indices $\langle 1, 1\rangle$. So if $V(x)$ is not limit point at both ends, then H is not essentially self-adjoint.

Now, suppose that $V(x)$ is limit point at both ends. For $f, g \in D(H^*)$, we set $W_x(f, g) = \overline{f(x)}g'(x) - \overline{f'(x)}g(x)$. W_x is continuous and

$$W_b(f, g) - W_a(f, g) = \int_a^b [\overline{(H^*f)(x)}g(x) - \overline{f(x)}(H^*g)(x)]\, dx$$

by integration by parts. Since the integrand on the right-hand side is in $L^1(0, \infty)$, the limits $W_\infty(f, g) = \lim_{b\to\infty} W_b(f, g)$ and $W_0(f, g) = \lim_{a\to 0} W_a(f, g)$ exist and

$$W_\infty(f, g) - W_0(f, g) = (H^*f, g) - (f, H^*g)$$

If we can show that the left-hand side is zero, then H^* is symmetric and therefore H is essentially self-adjoint.

Choose $c \in (0, \infty)$. Let B be the restriction of H to $C_0^\infty(0, c) \subset L^2(0, c)$ and let A be $-d^2/dx^2 + V(x)$ on

$$D(A) = \{\varphi \mid \varphi \in C^\infty(0, c),\ \varphi = 0 \text{ near zero},\ \varphi(c) = 0\}$$

Since $B \subset A$, we have $\overline{B} \subset \overline{A}$. But there are functions in $D(\overline{A})$ with $\varphi'(c) \neq 0$ and no such functions are in $D(\overline{B})$ so $\overline{A}$ is a *proper* closed symmetric extension of $\overline{B}$. Since both solutions of $-\varphi'' + V\varphi = \pm i\varphi$ are L^2 near c, but only one is L^2 near zero, the deficiency indices of B are $\langle 1, 1\rangle$. Therefore, the deficiency indices of $\overline{A}$ are $\langle 0, 0\rangle$, so $\overline{A}$ is self-adjoint.

Now, let $f, g \in D(H^*)$ and choose $f_1, g_1 \in C_0^\infty(0, \infty)$ be such that $f(c) + f_1(c) = 0$, $g(c) + g_1(c) = 0$. Set $f_2 = f + f_1$, $g_2 = g + g_1$. Then

$$\begin{aligned} -W_0(f, g) &= W_c(f_2, g_2) - W_0(f_2, g_2) \\ &= (\overline{A}f_2, g_2) - (f_2, \overline{A}g_2) = 0 \end{aligned}$$

since $f_2, g_2 \in D(A^*) = D(\overline{A})$. Thus, $W_0(f, g) = 0$ and a similar proof shows that $W_\infty(f, g) = 0$. ∎

We now want to investigate when $V(x)$ is in the limit point case at both ends. The discussion in Examples 1 and 2 of Section 1 suggests that H will be essentially self-adjoint if and only if in the classical motion generated by $V(x)$ the particle stays away from 0 and ∞ so that we need not specify boundary conditions at zero or infinity (we will see presently to what extent this classical–quantum analogy holds). We define:

Definition The potential $V(x)$ is called **quantum-mechanically complete** if $H = -d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(0, \infty)$. $V(x)$ is said to be **complete at ∞** (respectively **at 0**) if at least one solution of $\varphi''(x) = V(x)\varphi(x)$ is not in L^2 near ∞ (respectively near 0).

In Example 2 of Section 1 we showed that the potential $V(x) \equiv 0$ is not complete. This is not surprising since a classical particle in a zero potential which starts out moving to the left will get to zero in finite time.

First we discuss the case at ∞. The standard sufficient condition is:

Theorem X.8 Let $V(x)$ be a continuous real-valued function on $(0, \infty)$ and suppose that there exists a positive differentiable function $M(x)$ so that

(i) $V(x) \geq -M(x)$

(ii) $\int_1^\infty (M(x))^{-1/2}\, dx = \infty$

(iii) $M'(x)/(M(x))^{3/2}$ is bounded near ∞.

Then $V(x)$ is in the limit point case (complete) at ∞.

Proof We will show that both solutions of $-\varphi'' + V\varphi = 0$ cannot be in L^2 near ∞. If $0 < c_1 < c < \infty$ and u is a real solution in L^2 near ∞, then

$$-K_1 \equiv -\int_{c_1}^\infty u^2(x)\, dx \leq -\int_{c_1}^c u^2(x)\, dx \leq \int_{c_1}^c \frac{V(x)}{M(x)}\, u^2(x)\, dx$$

$$= \int_{c_1}^c \frac{u''(x)u(x)}{M(x)}\, dx$$

An integration by parts then proves that u satisfies

$$-\frac{u'(x)u(x)}{M(x)}\Bigg]_{c_1}^c + \int_{c_1}^c \frac{(u'(x))^2}{M(x)}\, dx - \int_{c_1}^c \frac{u'(x)u(x)M'(x)\, dx}{(M(x))^2} \leq K_1 \quad \text{(X.13)}$$

for all c. Using hypothesis (iii) we can find K_2 so that

$$\int_{c_1}^c \frac{u'(x)u(x)M'(x)}{(M(x))^2}\, dx \leq K_2 \left(\int_{c_1}^c \frac{(u'(x))^2}{M(x)}\, dx\right)^{1/2} \left(\int_{c_1}^c (u(x))^2\, dx\right)^{1/2}$$

Suppose that $\int_{c_1}^\infty ((u'(x)^2/M(x))\, dx = \infty$. Then by the last inequality, the hypothesis on u, and (X.13), $u'(x)u(x)$ is positive near ∞. But, this would imply that $u'(x)$ and $u(x)$ always have the same sign, which is impossible because since u is in L^2 near infinity. Thus, $\int_{c_1}^\infty ((u'(x)^2/M(x))\, dx < \infty$.

Now suppose that φ and ψ are independent solutions of $-\varphi'' + V\varphi = 0$ which are in L^2 near infinity. We may assume that φ and ψ are real-valued and that they are normalized so that $\varphi(x)\psi'(x) - \varphi'(x)\psi(x) = 1$. Then,

$$\left(\frac{1}{M(x)}\right)^{1/2} = \frac{\varphi(x)\psi'(x)}{(M(x))^{1/2}} - \frac{\varphi'(x)\psi(x)}{(M(x))^{1/2}}$$

would be in L^1 near infinity which contradicts hypothesis (ii). ∎

Corollary Let $V(x)$ be differentiable on $(0, \infty)$ and bounded above by K on $[1, \infty)$. Suppose that

(i) $\int_1^\infty \frac{dx}{\sqrt{K - V(x)}} = \infty$.

(ii) $V'(x)|V(x)|^{-3/2}$ is bounded near infinity.

Then $V(x)$ is in the limit point case at ∞.

Thus if $V(x)$ is classically complete at ∞ (condition (i)) and in addition satisfies condition (ii), then $V(x)$ is quantum-mechanically complete. Condition (ii) says essentially that the derivative of V should not be too large compared to V. The following two examples show that on physical as well as mathematical grounds the classical and quantum problems will not be equivalent if the derivative of V is too large.

Example 1 (V is quantum-mechanically complete but classically incomplete at ∞) The potential $V(x)$ will be a series of steps smoothly connected on very short intervals (α_i, β_i) (see Figure X.2). It is clear that $\int_0^\infty (1/\sqrt{-V(x)})\, dx < \infty$, so the classical motion is incomplete at ∞. We will show that if the steps are sharp enough, the quantum motion is complete at infinity. The physical reason for this behavior is that part of the quantum-mechanical wave is reflected at each of the sharp steps and the steps are arranged so that the reflected waves are coherent. To see the idea of the proof, consider the case of infinitely sharp steps when $\alpha_k = k = \beta_k$. Let $\varphi(x) = -\cos(n^2\pi x - \frac{1}{2}n(n-1)\pi)$ for $n - 1 \leq x \leq n$. Then $\varphi \in D(H^*)$, $\varphi'' = V\varphi$, and $\varphi \notin L^2$ near infinity. We now show that we can smooth out this infinitely sharp step potential so that one solution of

$$\varphi''(x) = V(x)\varphi(x) \quad \text{(X.14)}$$

remains not in $L^2(0, \infty)$.

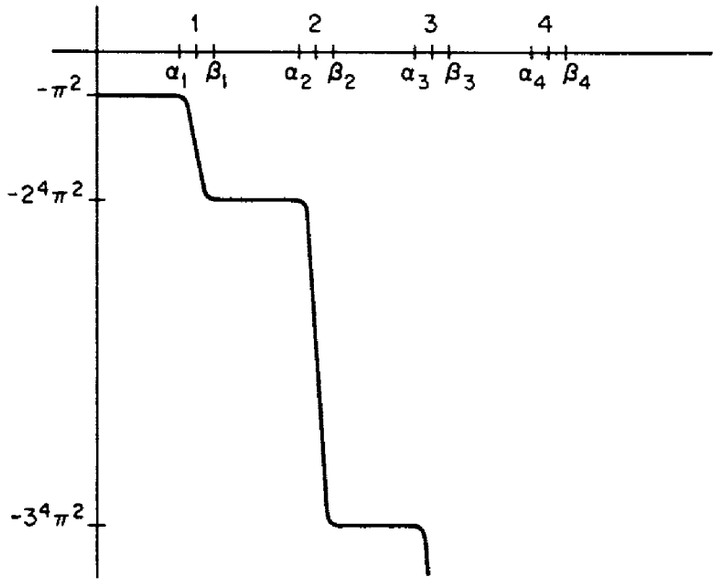


FIGURE X.2 The graph of V.

On the short intervals (α_k, β_k), V will be monotone decreasing in such a way that V is twice continuously differentiable. We take $\alpha_1 = 1$ and let $\varphi(x) = -\cos(\pi x)$ on $(0, 1]$. At $x = 1$, $\varphi(1) = 1$ and $\varphi'(1) = 0$. We want to pick β_1 so that the solution has not descended much at β_1. Since $V(x) < 0$, the solution will be concave downward until the next zero of $\varphi(x)$, call it r_1. On the interval $I_1 = (1, \min\{r_1, \alpha_2\})$, $\varphi(x)$ satisfies

$$\varphi(x) - 1 = \int_1^x \left(\int_1^s V(t)\varphi(t)\, dt \right) ds \tag{X.15}$$

which implies that

$$|\varphi(x) - 1| \leq \frac{(x-1)^2}{2} \left(\sup_{I_1} |V(t)| \right) \left(\sup_{I_1} |\varphi(t)| \right)$$
$$\leq \frac{(x-1)^2}{2} (2^4\pi^2)$$

We choose β_1 so that $|\varphi(\beta_1) - 1| \leq \frac{1}{4}$. Now we can put in the potential on the interval (α_1, β_1): the point is that whichever smooth connection we choose, the above a priori estimate guarantees that $\varphi(\beta_1) \geq 1 - \frac{1}{4}$. On (β_1, α_2), $\varphi(x)$ has the form $\varphi_2(x) = A_2 \cos(2^2\pi x - \gamma_2)$ where $|A_2| \geq 1 - \frac{1}{4}$. Now, choose α_2 to be the closest point to $x = 2$ where φ_2 has a maximum. We choose β_2 (using the same idea as above) so that $\varphi(\beta_2) \geq 1 - \frac{1}{4} - \frac{1}{8}$.

We proceed in this way to construct a solution $\varphi(x)$ which is

$$A_n \cos(n^2\pi x - \gamma_n)$$

on (β_{n-1}, α_n) with $|A_n| \geq \frac{1}{2}$. Thus $\varphi \notin L^2(0, \infty)$ so by Theorem X.6, V is in the limit point case at ∞.

Example 2 (V is classically complete but quantum-mechanically incomplete at ∞) Our potential will be of the form

$$V(x) = \frac{1}{x^2} - x^4 + \sum_{k=1}^{\infty} \sigma_k(x)$$

where the σ_k are very narrow smooth spikes of increasing height so that $V(k) = k$ (see Figure X.3). Since V is not bounded from above at ∞, the motion is classically complete. It follows from Theorem X.9 (below) that the potential $V_1(x) = x^{-2} - x^4$ is not quantum-mechanically complete at ∞, so that the corresponding Hamiltonian H_1 is not essentially self-adjoint on $C_0^\infty(0, \infty)$. We will use a perturbation method from Section X.2 to show that $H = H_1 + \sum \sigma_k(x)$ is similarly not essentially self-adjoint on $C_0^\infty(0, \infty)$ if the spikes σ_k are narrow enough. Since the potential $V = V_1 + \sum \sigma_k$ is limit point at zero by Theorem X.10 (below), it must be limit circle at infinity. The physical reason for this behavior is that if the spikes are narrow enough, the quantum particle can tunnel through them even though the classical particle is turned back.

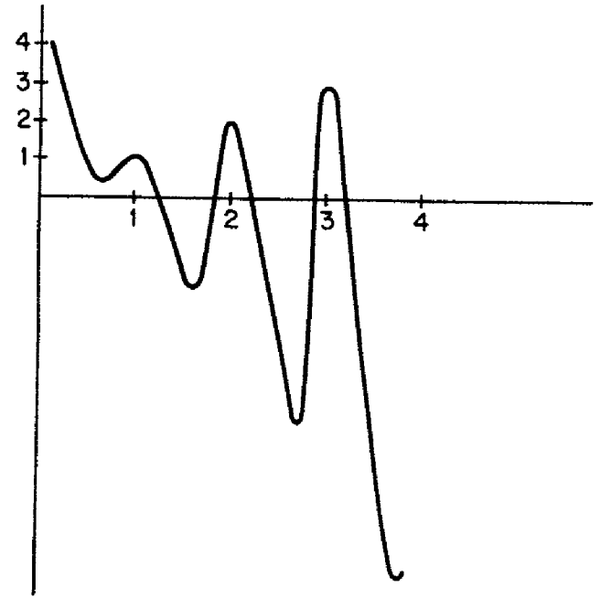


FIGURE X.3 The graph of V.

To prove that H is not essentially self-adjoint, we will show that, in the language of Section X.2, $\sum \sigma_k$ is $(-d^2/dx^2 + V_1)$-bounded with bound less than one on $C_0^\infty(0, \infty)$. That is, for some $a < 1$,

$$\|(\textstyle\sum \sigma_k)\varphi\|^2 \leq a^2\|-\varphi'' + V_1\varphi\|^2 + b^2\|\varphi\|^2 \tag{X.16}$$

for all $\varphi \in C_0^\infty(0, \infty)$. By the symmetric form of the Kato–Rellich theorem (Theorem X.13), this implies that $-d^2/dx^2 + V_1$ and $-d^2/dx^2 + V_1 + \sum \sigma_k$ are either both essentially self-adjoint or both not essentially self-adjoint on $C_0^\infty(0, \infty)$.

To prove (X.16) we use the following Sobolev-type estimate which the reader is asked to prove in Problem 10. Let $x_0 \in \mathbb{R}$, $\varphi \in C_0^\infty(\mathbb{R})$, and let $I_4^y = \{x \mid |x - y| \leq \frac{1}{4}\}$ and $I_2^y = \{x \mid |x - y| \leq \frac{1}{2}\}$. Then there is a constant C, independent of φ and y, so that

$$\sup_{x \in I_4^y} |\varphi|^2 \leq C(\|\varphi''\|^2_{L^2(I_2^y)} + \|\varphi\|^2_{L^2(I_2^y)}) \tag{X.17}$$

Let $\sigma_k(x) \in C_0^2(I_4^k)$ be such that $V_1(x) + \sigma_k(x)$ reaches its maximum in I_4^k at k and the value at the maximum is k. Let $\varepsilon(k)$ denote the diameter of the support of $\sigma_k(x)$. Then for $\varphi \in C_0^\infty(\mathbb{R})$,

$$\begin{aligned}\|\sigma_k\varphi\|^2 &\leq 4\varepsilon(k)k^8 \sup_{I_4^k} |\varphi|^2 \\ &\leq 4\varepsilon(k)k^8(\|\varphi''\|^2_{L^2(I_2^k)} + \|\varphi\|^2_{L^2(I_2^k)}) \\ &\leq 8\varepsilon(k)k^8[\|-\varphi'' + V_1\varphi\|^2_{L^2(I_2^k)} + \|V_1\varphi\|^2_{L^2(I_2^k)} + \|\varphi\|^2_{L^2(I_2^k)}]\end{aligned}$$

since $\|\psi_1\|^2 \leq \|\psi_1\|^2 + \|\psi_1 + 2\psi_2\|^2 = 2\|\psi_1 + \psi_2\|^2 + 2\|\psi_2\|^2$. Now, choose $\varepsilon(k)$ so small that $8\varepsilon(k)k^8 \leq \frac{1}{2}$ and $\sup_{x \in I_2^k} |16\varepsilon(k)k^8 V_1(x)| \leq 1$. Then

$$\begin{aligned}\left\| \sum_{k=1}^{\infty} \sigma_k \varphi \right\|^2 &= \sum_{k=1}^{\infty} \|\sigma_k\varphi\|^2 \\ &\leq \sum_{k=1}^{\infty} (\tfrac{1}{2}\|-\varphi'' + V_1\varphi\|^2_{L^2(I_2^k)} + 2\|\varphi\|^2_{L^2(I_2^k)}) \\ &\leq \tfrac{1}{2}\|-\varphi_1'' + V_1\varphi\|^2 + 2\|\varphi\|^2\end{aligned}$$

This completes the proof of (X.16).

The following theorem shows that if the derivatives of V are not too large compared to V itself, then V is classically complete at ∞ if and only if it is quantum-mechanically complete at ∞ (for the proof, see the references in the Notes).

Theorem X.9 Let V be a twice continuously differentiable real-valued function on $(0, \infty)$ and suppose that $V(x) \to -\infty$ as $x \to \infty$. Suppose further that

$$\int_c^\infty \left(\frac{[(-V)^{1/2}]'}{(-V)^{3/2}}\right)'(-V)^{-1/4}\,dx < \infty$$

for some c. Then V is in the limit point case at ∞ if and only if $\int_c^\infty (-V(x))^{-1/2}\,dx = \infty$, i.e., if and only if V is classically complete at ∞.

Example 3 Let $c > 0$. One easily concludes from this theorem that $-d^2/dx^2 - cx^\alpha$ is in the limit point case at ∞ if and only if $\alpha \leq 2$. For further discussion of this example, see Section X.5.

We turn now to the question of completeness at zero. There is a wide variety of theorems which guarantee either the limit point or limit circle case at zero. The following theorem gives conditions for positive potentials.

Theorem X.10 Let V be continuous and *positive* near zero. If $V(x) \geq \frac{3}{4}x^{-2}$ near zero then $-d^2/dx^2 + V(x)$ is in the limit point case at zero. If for some $\varepsilon > 0$, $V(x) \leq (\frac{3}{4} - \varepsilon)x^{-2}$ near zero, then $-d^2/dx^2 + V(x)$ is in the limit circle case.

Proof We deal first with the case where $V(x) = c/x^2$, $c > 0$. Two independent solutions of the equation $-\varphi''(x) + (c/x^2)\varphi(x) = 0$ are x^{α_1} and x^{α_2} where $\alpha_1 = (1 + \sqrt{1 + 4c})/2$ and $\alpha_2 = (1 - \sqrt{1 + 4c})/2$. x^{α_1} is always in L^2 near zero but x^{α_2} is in L^2 near zero if and only if $\alpha_2 > -\frac{1}{2}$, i.e., if and only if $c < \frac{3}{4}$. Thus $-\varphi''(x) + (c/x^2)\varphi(x) = 0$ has two independent solutions in L^2 near zero if and only if $c < \frac{3}{4}$.

We now prove the theorem by a comparison argument. Suppose that V and $\tilde{V}$ are both positive on an interval $(0, b)$ and $V(x) \geq \tilde{V}(x)$. Suppose $A > 0$ and let u_A be a solution of $u''(x) = V(x)u(x)$ satisfying $u(b/2) = 2$, $u'(b/2) = -A$, and let $\tilde{u}_A$ be a solution of $u''(x) = \tilde{V}(x)u(x)$ satisfying $\tilde{u}(b/2) = 1$, $\tilde{u}'(b/2) = -A/2$. A short argument shows that $u_A(x) > \tilde{u}_A(x)$ for all $x \in (0, b/2)$. Choosing A to be two different positive numbers we get two independent solutions of the two equations respectively. This shows that if $\tilde{u}''(x) = \tilde{V}(x)\tilde{u}(x)$ has a solution which is not L^2 near zero, then so does $u''(x) = V(x)u(x)$. Thus, if $-d^2/dx^2 + \tilde{V}(x)$ is limit point near zero, then so

is $-d^2/dx^2 + V(x)$, and if $-d^2/dx^2 + V(x)$ is limit circle, then so is $-d^2/dx^2 + \tilde{V}(x)$. Combining these statements with the results when $V(x) = cx^{-2}$ proves the theorem. ∎

Another useful condition is that $-d^2/dx^2 + V(x)$ is limit circle at zero if $V(x)$ is decreasing as x goes to zero. The proof is outlined in Problem 7. As in the case at ∞ (Example 2), it is possible to construct a potential V so that V is classically incomplete at zero but quantum-mechanically complete.

The following example shows that information about problems on a half-line can be used in certain multidimensional problems.

Example 4 (spherically symmetric potentials) A potential on $\mathbb{R}^n$ which only depends on $r = (\sum_{i=1}^n x_i^2)^{1/2}$, the distance from the origin, is called spherically symmetric. Let $D = C_0^\infty(\mathbb{R}^n \backslash \{0\})$, the C^∞ functions with compact support away from the origin. We will investigate $-\Delta + V(r)$ on D. We may regard each $\varphi \in L^2(\mathbb{R}^n)$ as a function of r and $n-1$ variables ξ on the sphere S^{n-1}. In terms of these variables

$$\|f\|_2^2 = \int_0^\infty \left(\int_{S^{n-1}} |f(r, \xi)|^2 \, d\Omega \right) r^{n-1} \, dr$$

where $d\Omega$ is the usual area measure on the sphere. Let $\tilde{D}$ be the set of functions in D which are finite linear combinations of products $f(r)g(\xi)$. $\tilde{D}$ is also dense in $L^2(\mathbb{R}^n)$ by Theorem II.10 since $L^2(\mathbb{R}^n) = L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes L^2(S^{n-1}, d\Omega)$. On functions of the form $f(r)g(\xi)$, $-\Delta + V(r)$ acts by

$$(-\Delta + V(r))f(r)g(\xi) = \left(-\frac{d^2}{dr^2} + V(r) - \frac{n-1}{r}\frac{d}{dr} \right) f(r)g(\xi) - \frac{1}{r^2} f(r) B g(\xi)$$

where B is the Laplace–Beltrami operator on $L^2(S^{n-1})$. It turns out (see the Notes) that B is essentially self-adjoint and negative on $C^\infty(S^{n-1})$, has only point spectrum of finite multiplicity, and that the corresponding eigenfunctions are C^∞. We will denote by K_ℓ the eigenspace corresponding to the ℓth eigenvalue κ_ℓ (we list the eigenvalues in decreasing order starting with $\kappa_0 = 0$). Then

$$L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes L^2(S^{n-1}, d\Omega) = \bigoplus_{\ell=0}^{\infty} L_\ell$$

where

$$L_\ell = L^2(\mathbb{R}^+, r^{n-1}\,dr) \otimes K_\ell$$

Define $D_\ell = \tilde{D} \cap L_\ell$, then

$$(-\Delta + V(r)) \restriction D_\ell = \left(-\frac{d^2}{dr^2} - \frac{n-1}{r}\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2} \right) \otimes I$$

By Theorem VIII.33 and Problem 1a, to conclude that $-\Delta + V(r)$ is essentially self-adjoint on $\tilde{D}$ and therefore on D, we need only prove that for each ℓ,

$$-\frac{d^2}{dr^2} - \left(\frac{n-1}{r}\right)\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^+) \subset L^2(\mathbb{R}^+, r^{n-1}\,dr)$.

Let $U\colon L^2(\mathbb{R}^+, r^{n-1}\,dr) \to L^2(\mathbb{R}^+, dr)$ be the unitary operator $U\colon \varphi(r) \mapsto r^{(n-1)/2}\varphi(r)$. U takes $C_0^\infty(\mathbb{R}^+)$ into itself and

$$U\left(-\frac{d^2}{dr^2} - \frac{n-1}{r}\frac{d}{dr} + V(r) - \frac{\kappa_\ell}{r^2} \right) U^{-1}$$

$$= -\frac{d^2}{dr^2} + V(r) + \left(\frac{(n-1)(n-3)}{4} - \kappa_\ell \right) \frac{1}{r^2} \tag{X.18a}$$

Each κ_ℓ is less than or equal to zero, so by Theorem X.10, each of these operators will be essentially self-adjoint on $C_0^\infty(\mathbb{R}^+)$ if

$$V(r) + \frac{(n-1)(n-3)}{4}\frac{1}{r^2} \geq \frac{3}{4r^2} \tag{X.18b}$$

On the other hand, if

$$0 \leq V(r) + \frac{(n-1)(n-3)}{4}\frac{1}{r^2} \leq \frac{c}{r^2}, \qquad c < \frac{3}{4} \tag{X.18c}$$

then one or more of the operators in (X.18a) will not be essentially self-adjoint on $C_0^\infty(\mathbb{R}^+)$. Thus, we have proven the following theorem:

Theorem X.11 Let $V(r)$ be a continuous symmetric potential on $\mathbb{R}^n \backslash \{0\}$. If $V(r)$ satisfies (X.18b), then $-\Delta + V(r)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$. If $V(r)$ satisfies (X.18c), then $-\Delta + V(r)$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$.

We remark that this theorem shows in particular that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$ if and only if $n \geq 4$. This fact is somewhat subtle if $n = 4$ but can be more easily proven if $n \geq 5$ (Problem 9). The first half of Theorem X.11 has a generalization to the noncentral case; see Section X.4.

X.2 Perturbations of self-adjoint operators

In this section we will prove several theorems which say that if A is self-adjoint and B is not too large compared to A, then $A + B$ is self-adjoint. These theorems have fundamental applications in quantum mechanics. First we define what we mean by a "small" perturbation.

Definition Let A and B be densely defined linear operators on a Hilbert space $\mathscr{H}$. Suppose that:

(i) $D(B) \supset D(A)$

(ii) For some a and b in $\mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\| \tag{X.19a}$$

Then B is said to be **A-bounded**. The infimum of such a is called the **relative bound** of B with respect to A. If the relative bound is zero, we say that B is **infinitesimally small** with respect to A and write $B << A$. We remark that usually b must be chosen larger as a is chosen smaller.

Sometimes, it is convenient to replace (ii) in the above definition by

(iii) For some $\tilde{a}, \tilde{b} \in \mathbb{R}$ and all $\varphi \in D(A)$,

$$\|B\varphi\|^2 \leq \tilde{a}^2\|A\varphi\|^2 + \tilde{b}^2\|\varphi\|^2 \tag{X.19b}$$

If (iii) holds, then (ii) holds with $a = \tilde{a}$, $b = \tilde{b}$. And if (ii) holds, we can conclude that (iii) holds with $\tilde{a}^2 = (1 + \varepsilon)a^2$, $\tilde{b}^2 = (1 + \varepsilon^{-1})b^2$ for each $\varepsilon > 0$. Thus, the infimum over all a in (ii) is equal to the infimum over all $\tilde{a}$ in (iii). Note that to prove estimates of the form (ii) or (iii) it is sufficient to prove them on a core for A.

A fundamental perturbation result is:

Theorem X.12 (the Kato–Rellich theorem) Suppose that A is self-adjoint, B is symmetric, and B is A-bounded with relative bound $a < 1$. Then $A + B$ is self-adjoint on $D(A)$ and essentially self-adjoint on any core of A. Further, if A is bounded below by M, then $A + B$ is bounded below by $M - \max\{b/(1 - a), a|M| + b\}$ where a and b are given by (X.19a).

Proof We will show that $\mathrm{Ran}(A + B \pm i\mu_0) = \mathscr{H}$ for some $\mu_0 > 0$. For $\varphi \in D(A)$, we have

$$\|(A + i\mu)\varphi\|^2 = \|A\varphi\|^2 + \mu^2\|\varphi\|^2$$

Letting $\varphi = (A + i\mu)^{-1}\psi$, we conclude from this that $\|A(A + i\mu)^{-1}\| \leq 1$ and $\|(A + i\mu)^{-1}\| \leq \mu^{-1}$. Therefore, applying (X.19a) with $\varphi = (A + i\mu)^{-1}\psi$, we find that

$$\|B(A + i\mu)^{-1}\psi\| \leq a\|A(A + i\mu)^{-1}\psi\| + b\|(A + i\mu)^{-1}\psi\|$$
$$\leq \left(a + \frac{b}{\mu}\right)\|\psi\|$$

Thus, for μ_0 large, $C = B(A + i\mu_0)^{-1}$ has norm less than one, since $a < 1$. This implies that $-1 \notin \sigma(C)$, so $\mathrm{Ran}(I + C) = \mathscr{H}$. Since A is self-adjoint, $\mathrm{Ran}(A + i\mu_0) = \mathscr{H}$ also. Thus the equation

$$(I + C)(A + i\mu_0)\varphi = (A + B + i\mu_0)\varphi \qquad \text{for} \quad \varphi \in D(A)$$

implies that $\mathrm{Ran}(A + B + i\mu_0) = \mathscr{H}$. The proof that $\mathrm{Ran}(A + B - i\mu_0) = \mathscr{H}$ is the same. Thus, by the fundamental criterion (Theorem VIII.3), $A + B$ is self-adjoint on $D(A)$.

It is a direct consequence of (X.19) that $D(\overline{(A + B) \restriction D_0}) \supset D(\overline{A \restriction D_0})$, so $A + B$ is essentially self-adjoint on any core of A.

Finally we prove the semiboundedness statement. Suppose that $t \in \mathbb{R}$ and $-t < M$. Then $\mathrm{Ran}(A + t) = \mathscr{H}$ and the same estimates as before show that $\|B(A + t)^{-1}\| < 1$ if

$$-t < M - \max\left\{\frac{b}{1 - a}, a|M| + b\right\}$$

Thus for such t, $\mathrm{Ran}(A + B + t) = \mathscr{H}$ and $(A + B + t)^{-1} = (A + t)^{-1} \times (I + C)^{-1}$ which implies that $-t \in \rho(A + B)$. ∎

The following symmetric form of the Kato–Rellich theorem is sometimes useful. For an application, see Example 3 in the Appendix to Section X.1.

Theorem X.13 Let A and C be symmetric operators. Suppose that D is a linear subspace satisfying $D \subseteq D(A)$, $D \subseteq D(C)$, and that

$$\|(A - C)\varphi\| \leq a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\|$$

for all $\varphi \in D$, where $a < 1$. Then,

(a) A is essentially self-adjoint on D if and only if C is essentially self-adjoint on D.

(b) $D(\overline{A \restriction D}) = D(\overline{C \restriction D})$.

Proof Let $B = A - C$ with $D(B) = D$ and define $F(\alpha) = C + \alpha B$ for $0 \le \alpha \le 1$. Then $F(0) = C, F(1) = A$ and $C\varphi = F(\alpha)\varphi - \alpha B\varphi, A\varphi = F(\alpha)\varphi + (1-\alpha)B\varphi$ for all $\varphi \in D$. Thus, the inequality in the hypothesis implies that

$$\begin{aligned}\|B\varphi\| &\le a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\| \\ &\le 2a\|F(\alpha)\varphi\| + a\|B\varphi\| + b\|\varphi\|\end{aligned}$$

or

$$\|B\varphi\| \le \frac{2a}{1-a}\|F(\alpha)\varphi\| + \frac{b}{1-a}\|\varphi\| \tag{X.20}$$

Let $0 \le \alpha' \le 1$. If $2a\alpha'/(1-a) < 1$, (X.20) and Theorem X.12 imply that $F(\alpha + \alpha') = F(\alpha) + \alpha' B$ is essentially self-adjoint on D if and only if $F(\alpha)$ is. Thus, starting with $\alpha = 0$ and applying this result finitely many times, we conclude (a). The reader is asked (Problem 13) to follow similar steps to prove (b). ∎

The following theorem extends Theorem X.12 to the case of relative bound one, but it has a slightly weaker conclusion.

Theorem X.14 (Wüst's theorem) Let A be self-adjoint and B be symmetric with $D(B) \supset D(A)$. Suppose that for some b and all $\varphi \in D(A)$,

$$\|B\varphi\| \le \|A\varphi\| + b\|\varphi\| \tag{X.21a}$$

Then $A + B$ is *essentially* self-adjoint on $D(A)$ or any core for A.

Proof By a simple argument, it is enough to show that $A + B$ is essentially self-adjoint on $D(A)$. Suppose that $(A + B + i)^* h = 0$. For each $t < 1$, $A + tB$ is self-adjoint on $D(A)$ by Theorem X.12. Thus, there exists $\varphi_t \in D(A)$ with $\|\varphi_t\| \le \|h\|$, so that $(A + tB + i)\varphi_t = h$. Define $\psi_t = h - (t-1)B\varphi_t$. Then a short calculation shows that $(\psi_t, h) = 0$. By (X.21a),

$$\begin{aligned}\|A\varphi_t\| &\le \|(A + tB)\varphi_t\| + \|tB\varphi_t\| \\ &\le \|(A + tB)\varphi_t\| + t\|A\varphi_t\| + tb\|\varphi_t\|\end{aligned}$$

so

$$(1-t)\|A\varphi_t\| \le \|(A + tB)\varphi_t\| + tb\|\varphi_t\|$$

Since $\|(A + tB)\varphi_t\|^2 = \|h\|^2 - \|\varphi_t\|^2$, this implies that $(1-t)\|A\varphi_t\|$ is bounded as $t \uparrow 1$. It follows by using (X.21a) again that $(1-t)\|B\varphi_t\|$ and therefore also $\|\psi_t\|$ are bounded as $t \uparrow 1$. Now let $\eta \in D(A)$. Then

$$\lim_{t \uparrow 1}(\psi_t - h, \eta) = \lim_{t \uparrow 1}(t-1)(\varphi_t, B\eta) = 0$$

Since the $\|\psi_t\|$ are uniformly bounded, we conclude that $h = w\text{-}\lim \psi_t$. But then $(h, h) = \lim(h, \psi_t) = 0$ so $h = 0$. We conclude that $\mathrm{Ker}(A + B + i)^* = \{0\}$. The proof that $\mathrm{Ker}(A + B - i)^* = \{0\}$ is similar. ∎

Choosing $A = -B$ shows that "essentially self-adjoint" cannot be replaced by "self-adjoint" in the statement of Theorem X.14. We also note that there are counterexamples which show that the conclusion of the theorem may be false if the relative bound is larger than one. (See Example 4 at the end of this section.) We also note that according to our discussion of (X.19a) and (X.19b), the condition (X.21a) needed to apply Theorem X.14 is itself implied by the condition

$$\|B\varphi\|^2 \le \|A\varphi\|^2 + b^2\|\varphi\|^2 \tag{X.21b}$$

which is equivalent to the operator inequality

$$B^2 \le A^2 + b^2 \tag{X.21c}$$

We come now to Kato's basic application of the Kato–Rellich theorem to atomic Hamiltonians. First, we define some new classes of functions.

Definition Let $\langle M, \mu\rangle$ be a measure space. The set of measurable functions f on M which can be written $f = f_1 + f_2$ where $f_1 \in L^r(M, d\mu)$ and $f_2 \in L^s(M, d\mu)$ will be denoted by $L^r(M, d\mu) + L^s(M, d\mu)$.

Theorem X.15 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ be real-valued. Then $-\Delta + V(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$ and self-adjoint on $D(-\Delta)$.

Proof Since V is real-valued, the operator of multiplication by V is self-adjoint on

$$D(V) = \{\varphi \,|\, \varphi \in L^2(\mathbb{R}^3), V\varphi \in L^2(\mathbb{R}^3)\}$$

Let $V = V_1 + V_2$ with $V_1 \in L^2(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. Then

$$\|V\varphi\|_2 \le \|V_1\|_2 \|\varphi\|_\infty + \|V_2\|_\infty \|\varphi\|_2 \tag{X.22}$$

so $D(V) \supset C_0^\infty(\mathbb{R}^3)$. By Theorem IX.28, given any $a > 0$, there is a $b > 0$ so that

$$\|\varphi\|_\infty \le a\|\Delta\varphi\|_2 + b\|\varphi\|_2 \tag{X.23}$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. This inequality and (X.22) give

$$\|V\varphi\|_2 \le a\|V_1\|_2 \|-\Delta\varphi\|_2 + (b + \|V_2\|_\infty)\|\varphi\|_2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^3)$. Thus V is $-\Delta$-bounded with arbitrarily small bound on $C_0^\infty(\mathbb{R}^3)$. Since $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, the Kato–Rellich theorem implies that $-\Delta + V$ is also essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 1 Let $V(r) = -e^2/r$ where $r = \sqrt{x^2 + y^2 + z^2}$. Then $-\Delta - e^2/r$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Theorem X.16 (Kato's theorem) Let $\{V_k\}_{k=1}^m$ be a collection of real-valued measurable functions each of which is in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Let $V_k(\mathbf{y}_k)$ be the multiplication operator on $L^2(\mathbb{R}^{3n})$ obtained by choosing $\mathbf{y}_k$ to be three coordinates of $\mathbb{R}^{3n}$. Then $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$, where Δ denotes the Laplacian on $\mathbb{R}^{3n}$.

Proof First we consider one of the functions V_k separately. By a rotation of variables we may assume the variables in $V_k(\cdot)$ are x_1, x_2, x_3. (This is because $\|\cdot\|_2$, $\|\cdot\|_\infty$, and $-\Delta$ are invariant under rotations of coordinates.) Let Δ_1 denote the Laplacian with respect to x_1, x_2, x_3. By the estimate (X.23), together with the "equivalence" of the bounds (X.19a) and (X.19b), we have for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$,

$$\begin{aligned}
\|V_k\varphi\|^2_{L^2(\mathbb{R}^{3n})} &\le a^2 \int |-\Delta_1\varphi(x_1, \ldots, x_{3n})|^2 \, dx_1 \cdots dx_{3n} \\
&\quad + b^2 \int |\varphi(x_1, \ldots, x_{3n})|^2 \, dx_1 \cdots dx_{3n} \\
&= a^2 \int \left| \sum_{i=1}^3 p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2\|\varphi\|^2 \\
&\le a^2 \int \left| \sum_{i=1}^n p_i^2 \hat{\varphi}(p_1, \ldots, p_{3n}) \right|^2 dp_1 \cdots dp_{3n} + b^2\|\varphi\|^2 \\
&= a^2\|-\Delta\varphi\|^2 + b^2\|\varphi\|^2
\end{aligned}$$

Thus, using the Schwarz inequality, one easily concludes that

$$\left\| \sum_{k=1}^m V_k(\mathbf{y}_k)\varphi \right\|^2 \le m^2a^2\|-\Delta\varphi\|^2 + m^2b^2\|\varphi\|^2$$

for all $\varphi \in C_0^\infty(\mathbb{R}^{3n})$. Since a may be chosen as small as we like, we conclude that $\sum_{k=1}^m V_k(\mathbf{y}_k)$ is infinitesimally small with respect to $-\Delta$. Thus, by the Kato–Rellich theorem, $-\Delta + \sum_{k=1}^m V_k(\mathbf{y}_k)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. ∎

Example 2 (atomic Hamiltonians) Let $\mathbf{x}_1, \ldots, \mathbf{x}_n$ in $\mathbb{R}^3$ be orthogonal coordinates for $\mathbb{R}^{3n}$. Then

$$-\sum_{i=1}^n \Delta_i - \sum_{i=1}^n \frac{ne^2}{|\mathbf{x}_i|} + \sum_{i<j}^n \frac{e^2}{|\mathbf{x}_i - \mathbf{x}_j|}$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3n})$.

For an application of the Kato–Rellich theorem to ordinary differential operators, see Problem 7.

There is a form analogue of the Kato–Rellich theorem which can be used when the form $(B\varphi, \varphi)$ is "small" with respect to the form $(A\varphi, \varphi)$ even though B may not be A-bounded. Although the statement of the theorem below is similar to Theorem X.12, the proof is very different.

Theorem X.17 (the KLMN theorem) Let A be a positive self-adjoint operator and suppose that $\beta(\varphi, \psi)$ is a symmetric quadratic form on $Q(A)$ such that

$$|\beta(\varphi, \varphi)| \le a(\varphi, A\varphi) + b(\varphi, \varphi) \qquad \text{all } \varphi \in D(A) \tag{X.24}$$

for some $a < 1$ and $b \in \mathbb{R}$. Then there exists a unique self-adjoint operator C with $Q(C) = Q(A)$ and

$$(\varphi, C\psi) = (\varphi, A\psi) + \beta(\varphi, \psi) \qquad \text{all } \varphi, \psi \in Q(C)$$

C is bounded below by $-b$ and any domain of essential self-adjointness for A is a form core for C.

Proof Define a form $\gamma(\varphi, \psi) = (\varphi, A\psi) + \beta(\varphi, \psi)$ on $Q(A)$. By (X.24),

$$\begin{aligned}
\gamma(\varphi, \varphi) &\ge (1 - a)(\varphi, A\varphi) - b(\varphi, \varphi) \\
&\ge -b(\varphi, \varphi)
\end{aligned}$$

since A is positive. Thus γ is bounded from below by $-b$. Furthermore

$$\begin{aligned}
(1 - a)(\varphi, A\varphi) + (\varphi, \varphi) &\le \gamma(\varphi, \varphi) + (b + 1)(\varphi, \varphi) \\
&\le (1 + a)(\varphi, A\varphi) + (2b + 1)(\varphi, \varphi)
\end{aligned}$$

Thus the $\|\cdot\|_{+1,A}$ and $\|\cdot\|_{+1,\gamma}$ norms are equivalent on $Q(A)$. Since $Q(A)$ is closed under $\|\cdot\|_{+1,A}$, it is closed under $\|\cdot\|_{+1,\gamma}$. Thus γ is a semi-bounded, closed quadratic form on $Q(A)$. The theorem now follows from the statement and proof of Theorem VIII.15. ∎

This theorem suggests that we define:

Definition Let A be a positive self-adjoint operator. Suppose that B is a self-adjoint operator which satisfies:

(i) $Q(B) \supset Q(A)$
(ii) $|(\varphi, B\varphi)| \leq a(\varphi, A\varphi) + b(\varphi, \varphi), \varphi \in Q(A)$

for some $a > 0$ and $b \in \mathbb{R}$. Then B is said to be **relatively form-bounded** with respect to A. If a can be chosen arbitrarily small, B is said to be **infinitesimally form-bounded** with respect to A (written $B \prec\prec A$).

If B is self-adjoint and relatively form-bounded ($a < 1$) with respect to a positive self-adjoint operator A, then the KLMN theorem gives meaning to $A + B$. We emphasize that this definition of "$A + B$" may *differ* from the operator sum. There are examples where B is relatively form-bounded with respect to A even though $D(A) \cap D(B) = \{0\}$. In fact, as the following example shows, the form β in the KLMN theorem need not be a form arising from an operator or even a closable form.

Example 3 Let $A = -d^2/dx^2$ on $\mathbb{R}$ and define $\beta(\varphi, \psi) = \overline{\varphi}(0)\psi(0)$ for $\varphi, \psi \in C_0^\infty(\mathbb{R})$. By Sobolev's lemma, for any $a > 0$, there is a b so that

$$\|\varphi\|_\infty^2 \leq a(\varphi, -\varphi'') + b\|\varphi\|^2$$

Thus we can apply the KLMN theorem to define $-d^2/dx^2 + \delta$! A function $\psi \in Q(-d^2/dx^2) \subset C_\infty(\mathbb{R})$ is in the domain of $-d^2/dx^2 + \delta$ if and only if $-\psi''(x) + \delta(x)\psi(0) \in L^2(\mathbb{R})$ where the derivative is taken in the sense of distributions. For example, if $\psi(x)$ looks like $1 + \frac{1}{2}|x|$ near zero and is C^∞ away from zero with compact support, then $\psi \in D(-d^2/dx^2 + \delta(x))$, since the $\delta(x)\psi(0)$ will just cancel the term $-\delta(x)\psi(x)$ which appears in $-\psi''(x)$. Thus, $D(A + B)$ can contain vectors which are neither in $D(A)$ nor in $D(B)$ but for which there are cancellations in "$A\psi + B\psi$."

The following theorem shows that if B is A-bounded, then B is form-bounded with respect to A.

Theorem X.18 Let A be a positive self-adjoint operator and suppose that B is self-adjoint. Then

(a) If B is A-bounded with relative bound a, then B is form-bounded with respect to A with relative bound a.
(b) $B << A$ implies $B \prec\prec A$.

Proof Let $C^\infty(A) = \bigcap_{n=1}^\infty D(A^n)$, $\mu > 0$, and let $\mathscr{H}_n$ be the closure of $C^\infty(A)$ under the norm $\|\varphi\|_n = \|(A + I)^{n/2}\varphi\|$, $n = 0, \pm 1, \pm 2, \ldots$. Then a map C from $C^\infty(A)$ to $\mathscr{H}$ extends to be a bounded operator from $\mathscr{H}_m$ to $\mathscr{H}_{-n}$ if and only if $(A + I)^{-n/2}C(A + I)^{-m/2}$ is bounded on $C^\infty(A)$ in the usual operator norm.

If B is A-bounded with relative bound a, then $B(A + \mu I)^{-1}$ and $(A + \mu I)^{-1}B$ are bounded by $(a + b/\mu)$. The interpolation argument in Example 3 of the Appendix to Section IX.4 proves that

$$(A + \mu I)^{-1/2}B(A + \mu I)^{-1/2}$$

is also bounded by $a + (b/\mu)$ and it follows immediately that

$$(\varphi, B\varphi) \leq \left(a + \frac{b}{\mu}\right)(\varphi, (A + \mu I)\varphi)$$

for $\varphi \in D_\infty(A)$. Since $\mu > 0$ is arbitrary, parts (a) and (b) follow. ∎

The KLMN theorem can sometimes be used to define Hamiltonians when Rellich's theorem does not apply. To see that the $L^2 + L^\infty$ class of potentials does not include all "reasonable" potentials, we remark that it is venerable physical folklore that potentials of the form $V_\alpha(r) = -r^{-\alpha}$ produce reasonable quantum dynamics as long as $\alpha < 2$. But $V_\alpha \in L^2 + L^\infty$ only if $\alpha < \frac{3}{2}$! Thus we cannot use Rellich's theorem if $\frac{3}{2} \leq \alpha < 2$ (see Problem 14). However, we can use the KLMN theorem. First, we prove an estimate:

Lemma (the uncertainty principle lemma) Let $\psi \in C_0^\infty(\mathbb{R}^3)$. Then

$$\int_{\mathbb{R}^3} \frac{1}{4r^2}\,|\psi(\mathbf{r})|^2\,d\mathbf{r} \leq \int_{\mathbb{R}^3} |\nabla\psi(\mathbf{r})|^2\,d\mathbf{r}$$

Proof We may suppose that ψ is real-valued. Then,

$$\nabla(r^{+1/2}\psi) = r^{1/2}\nabla\psi + \tfrac{1}{2}r^{-3/2}\mathbf{r}\psi$$

Thus, if $r \neq 0$,

$$\begin{aligned}|\nabla\psi|^2 &= |r^{-1/2}\nabla(r^{1/2}\psi) - \tfrac{1}{2}r^{-2}\mathbf{r}\psi|^2 \\ &\geq -r^{-3/2}\psi\,\frac{\partial}{\partial r}\,(r^{1/2}\psi) + \frac{1}{4}\,r^{-2}|\psi|^2 \\ &= -\frac{1}{2r^2}\,\frac{\partial}{\partial r}\,(r|\psi|^2) + \frac{1}{4}\,r^{-2}|\psi|^2\end{aligned}$$

So,

$$\int |\nabla\psi|^2\, d\mathbf{r} \geq \int \frac{1}{4r^2}\,|\psi|^2\, d\mathbf{r} - \frac{1}{2}\int_0^\infty \frac{\partial}{\partial r}\int_{S_2} r|\psi|^2\, d\Omega\, dr$$

$$= \int \frac{1}{4r^2}\,|\psi|^2\, d\mathbf{r} \quad \blacksquare$$

Proposition If $\alpha < 2$, then $-r^{-\alpha} \prec\prec -\Delta$.

Proof Let $\varphi \in C_0^\infty$ and let $a > 0$ be given. Choose $\varepsilon > 0$ so that $1/r^\alpha \leq a/4r^2$ for all $r \leq \varepsilon$. Then

$$\int_{\mathbb{R}^3} \frac{1}{r^\alpha}\,|\varphi(\mathbf{r})|^2\, d\mathbf{r} = \int_{|\mathbf{r}|\leq\varepsilon} \frac{1}{r^\alpha}\,|\varphi(\mathbf{r})|^2\, d\mathbf{r} + \int_{|\mathbf{r}|>\varepsilon} \frac{1}{r^\alpha}\,|\varphi(\mathbf{r})|^2\, d\mathbf{r}$$

$$\leq a\int_{|\mathbf{r}|\leq\varepsilon} |\nabla\varphi(\mathbf{r})|^2\, d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{|\mathbf{r}|>\varepsilon} |\varphi(\mathbf{r})|^2\, d\mathbf{r}$$

$$\leq a\int_{\mathbb{R}^3} (-\Delta\varphi(\mathbf{r}))\overline{\varphi(\mathbf{r})}\, d\mathbf{r} + \frac{1}{\varepsilon^\alpha}\int_{\mathbb{R}^3} |\varphi(\mathbf{r})|^2\, d\mathbf{r} \quad \blacksquare$$

This proposition shows that for $\frac{3}{2} \leq \alpha < 2$, we can use the KLMN theorem to define $-\Delta - r^{-\alpha}$. $L^2 + L^\infty$ is the natural class of potentials associated with the Kato–Rellich theorem (see Problem 14). There is no completely natural class associated with the KLMN theorem.

Definition A measurable function V on $\mathbb{R}^3$ is called a **Rollnik potential** if

$$\|V\|_R^2 \equiv \int_{\mathbb{R}^3} \frac{|V(x)|\,|V(y)|}{|x-y|^2}\, d^3x\, d^3y < \infty$$

We denote the set of Rollnik potentials by R.

R turns out to be a vector space which is complete under the Rollnik norm $\|\cdot\|_R$. Moreover, by Sobolev's inequality (IX.19), $L^{3/2}(\mathbb{R}^3) \subset R$; in particular $r^{-\alpha} \in R + L^\infty$ if $\alpha < 2$. The analogue of the Kato theorem is:

Theorem X.19

(a) If $V \in R + L^\infty(\mathbb{R}^3)$, then $V \prec\prec -\Delta$

(b) If $V_i(\mathbf{r})$ and $V_{ij}(\mathbf{r})$ are all in $R + L^\infty$ and

$$V = \sum V_i(\mathbf{r}_i) + \sum_{i,j=1}^{N} V_{ij}(\mathbf{r}_i - \mathbf{r}_j)$$

on $\mathbb{R}^{3N}$, then $V \prec\prec -\Delta$.

For the proof, see the references in the Notes or Problem 17. We remind the reader again that the meaning given to $-\Delta + V$ by the KLMN Theorem *may* differ from the operator sum defined on $D(-\Delta) \cap D(V)$.

The problem of determining conditions on a potential on $\mathbb{R}^s$ so that $-\Delta + V$ is essentially self-adjoint has been extensively studied using Rellich's theorem and the KLMN theorem. The proofs of the necessary inequalities often use the L^p-estimates of Section IX.4 and the interpolation theorems and therefore the results are usually dependent on the dimension s. We present two examples below. For other theorems, see Section X.4 and the references in the Notes.

Theorem X.20 Let $s \geq 4$. If $V \in L^p(\mathbb{R}^s)$ for some $p > s/2$, then $V << -\Delta$.

Proof By Theorem IX.27, we know that if $u \in D(-\Delta)$ then

$$(1 + k^2)\hat{u}(k) \in L^2(\mathbb{R}^s)$$

Further, since $p > s/2$, $(1 + k^2)^{-1} \in L^p(\mathbb{R}^s)$, so by the Hölder inequality $\hat{u} \in L^q$ and

$$\|\hat{u}\|_q \leq \|(1 + k^2)^{-1}\|_p \|(1 + k^2)\hat{u}\|_2$$

where $q^{-1} = p^{-1} + \frac{1}{2}$. Therefore, by the Hansdorff–Young inequality $u \in L^r(\mathbb{R}^s)$ where $r^{-1} = \frac{1}{2} - p^{-1}$. Since $V \in L^p$, it follows from the Hölder inequality that $Vu \in L^2$. Thus, $D(V) \supset D(-\Delta)$ and

$$\begin{aligned}\|Vu\|_2 \leq \|V\|_p \|u\|_r &\leq \|V\|_p \|\hat{u}\|_q \\ &= \|V\|_p \|(1 + tk^2)^{-1}(1 + tk^2)\hat{u}\|_q \\ &\leq \|V\|_p \|(1 + tk^2)^{-1}\|_p \|(1 + tk^2)\hat{u}\|_2 \\ &\leq (\|V\|_p \|(1 + k^2)^{-1}\|_p) t^{-s/2p}(\|u\|_2 + t\|-\Delta u\|_2)\end{aligned}$$

Since $p > s/2$. this estimate shows that $V << -\Delta$. $\blacksquare$

The above theorem can be extended to the borderline case $p = s/2$ when $s \geq 5$, but in fact a stronger result is true.

Theorem X.21 (Strichartz's theorem) Let $s \geq 5$ and suppose $V \in L_w^{s/2}$. Then V is Δ-bounded with bound less than or equal to $C\|V\|_{s/2,\,w}$ where C depends only on s.

Proof It is sufficient to show that $\|V(I + \Delta)^{-1}\varphi\|_2 \leq C\|V\|_{s/2,\,w}\|\varphi\|_2$ for all $\varphi \in L^2(\mathbb{R}^s)$. Since $(I + \Delta)^{-1}\varphi = G * \varphi$ where G is the Fourier transform

of $(1 + p^2)^{-1}$ on $\mathbb{R}^s$, we need the properties of G established in Problems 49 or 50 of Chapter IX. Since $G(x)$ is exponentially decreasing at ∞ and $\overline{\lim}_{|x|\to 0} |x|^{s-2}|G(x)| < \infty$, we easily find that $\mu\{x \mid |G(x)| \geq t\}$ is bounded by $c_2 t^{s/s-2}$ for some $c_2 > 0$, where μ is Lebesgue measure. Thus, using the inequality in Problem 39 of Chapter IX, with $p = s/2$ and $q = 2$, we conclude that

$$\|V(G * \varphi)\|_2 \leq C_3 \|V\|_{s/2,\,w} \|G\|_{s/s-2,\,w} \|\varphi\|_2 \quad \blacksquare$$

Corollary Let μ denote Lebesgue measure on $\mathbb{R}^s$, $s \geq 5$. If $V(x)$ is a real-valued measurable function and

$$\lim_{t\to\infty} t^{s/2}\mu\{x \mid |V(x)| \geq t\} = 0$$

then $V << -\Delta$. In particular, if $V \in L^{s/2}(\mathbb{R}^s)$, then $V << -\Delta$.

Example 4 Let $s = 5$. From Theorems X.10 and X.11, it follows that $-\Delta + \alpha/r^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -1.25$. Further, $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$. The reader can easily check that $1/r^2 \in L_w^{5/2}(\mathbb{R}^5)$, so by Strichartz' theorem, α/r^2 is $-\Delta$-bounded. Thus, the closure of $-\Delta + \alpha/r^2 \upharpoonright C_0^\infty(\mathbb{R}^5\backslash\{0\})$ contains

$$(-\Delta + \alpha/r^2) \upharpoonright C_0^\infty(\mathbb{R}^5)$$

Therefore, in the case $\alpha < -1.25$, $-\Delta + \alpha/r^2$ is not even essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$.

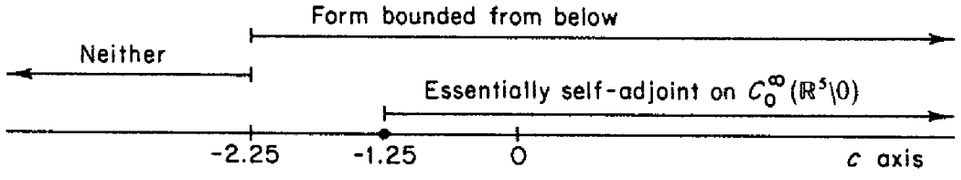


FIGURE X.4 The operator $-\Delta + (c/r^2)$ when $n = 5$.

In Problem 15, the reader is asked to show that $-d^2/dx^2 + c/x^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^+)$ if and only if $c \geq -\frac{1}{4}$. Thus, using the method of Example 4 of the Appendix to Section X.1, we conclude that $-\Delta + \alpha/r^2$ is form-bounded from below on $C_0^\infty(\mathbb{R}^5\backslash\{0\})$ if and only if $\alpha \geq -2.25$. Therefore, if α is in the range $-2.25 \leq \alpha < -1.25$, we can use the quadratic form techniques of Theorem VIII.15 to define $-\Delta + \alpha/r^2$, even though $-\Delta + \alpha/r^2$ is not essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$. See Figure X.4.

Example 5 (Schrödinger operators for systems with magnetic fields) According to the Lagrangian–Hamiltonian theory of classical mechanics, the energy operator written in terms of the coordinate $\mathbf{q}$ and the canonically conjugate momentum $\mathbf{p} = m\dot{\mathbf{q}} + e\mathbf{A}/c$ is

$$E = \frac{1}{2m}(\mathbf{p} - e\mathbf{A}/c)^2 + V(\mathbf{q})$$

where $\mathbf{A}$ is the **magnetic vector potential**, related to $\mathbf{B}$, the **magnetic field** by

$$\mathbf{B} = \nabla \times \mathbf{A} \tag{X.25}$$

Using the correspondence between classical energy functions and quantum-mechanical Hamiltonian operators (Section VIII.11), we see that the Hamiltonian for an n-particle system in the presence of a magnetic field is

$$H = \sum_{j=1}^{n} (2m_j)^{-1}\left(-i\nabla_j - \frac{e_j}{c}\mathbf{A}\right)^2 + V(\mathbf{x}_1, \ldots, \mathbf{x}_n) \tag{X.26}$$

The case

$$A(\mathbf{x}) = \tfrac{1}{2}\mathbf{x} \times \mathbf{B}_0 \tag{X.27}$$

with $\mathbf{B}_0$ constant is especially important for this leads to $\mathbf{B} = \mathbf{B}_0$. This constant field situation is called the Zeeman effect, and its treatment requires special methods (see Section 4) since A grows at infinity. For the present, we note that perturbation methods do allow the treatment of some kinds of magnetic vector potentials. We give a detailed version of the operator perturbation theory result and leave the form result to the reader (Problem 36):

Theorem X.22 Suppose that each component of $\mathbf{A}$ is a real-valued function in $L^4(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, that $\nabla \cdot \mathbf{A} \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (in the sense of distributions), and that V is a real-valued function in $L^2 + L^\infty$. For $\varphi \in C_0^\infty(\mathbb{R}^3)$, define

$$H\varphi = -\Delta\varphi + -2i\mathbf{A} \cdot \nabla\varphi - i(\nabla \cdot \mathbf{A})\varphi + V\varphi + A^2\varphi$$

Then H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$.

Proof Integration by parts shows that H is symmetric on $C_0^\infty(\mathbb{R}^3)$ and the hypotheses on V, A^2, and $\nabla \cdot \mathbf{A}$ were chosen so that, by Theorem X.15, we have $V << -\Delta$ and $\nabla \cdot \mathbf{A} << -\Delta$. We will show that $\mathbf{A} \cdot \nabla << -\Delta$,

which implies by Theorem X.12 that H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$. Let $\varphi \in C_0^\infty(\mathbb{R}^3)$. Suppose that $A \in L^4(\mathbb{R}^3)$. By the Hölder and Hausdorff–Young inequalities, we have

$$\begin{aligned}\left\| A^{(i)} \frac{\partial}{\partial x_i} \varphi \right\| &\leq \|A^{(i)}\|_4 \left\| \frac{\partial}{\partial x_i} \varphi \right\|_4 \\ &\leq \|A^{(i)}\|_4 \|p_i \hat{\varphi}(p)\|_{4/3} \\ &\leq \|A^{(i)}\|_4 \|(1+|p|)^{-\alpha}\|_4 \|(1+|p|)^{\alpha} p_i \hat{\varphi}(p)\|_2\end{aligned}$$

where we have chosen α to be any fixed number in $(\frac{3}{4}, 1)$. For any $a > 0$, there is a b so that

$$\begin{aligned}\|(1+|p|)^{\alpha} p_i \hat{\varphi}(p)\|_2 &\leq \|(b + a|p|^2)\hat{\varphi}(p)\|_2 \\ &\leq a\|\Delta\varphi\|_2 + b\|\varphi\|_2\end{aligned}$$

by the Plancherel theorem. Thus $A^{(i)}\, \partial/\partial x_i << -\Delta$. A separate proof works for the L^∞ part of A. ∎

Perturbation theorems are simple and elegant and are applicable in so many cases that the test of the usefulness of any other self-adjointness method is its applicability to situations that cannot be directly handled by Theorems X.12, X.14, or X.17. One of the simplest physically interesting examples of such a situation is the **anharmonic oscillator Hamiltonian** $-d/dx^2 + x^2 + x^4$, its analogues on $\mathbb{R}^s$, and more generally the operators $-d^2/dx^2 + x^2 + x^{2m}$ $(m = 2, 3, \ldots)$. Both $H_0 = -d^2/dx^2 + x^2$ and $V = x^4$ are essentially self-adjoint on $C_0^\infty(\mathbb{R})$, but neither is a small perturbation of the other. We will use $-d^2/dx^2 + x^2 + x^4$ as a test case for many of the self-adjointness methods which we discuss later; in fact, we present five distinct proofs that $-d^2/dx^2 + x^2 + x^4$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$! All these proofs extend to prove that

$$\sum_{i=1}^{n} a_i \left(-\frac{d^2}{dx_i^2} + \omega_i^2 x_i^2 \right) + \sum_{i,j,k,\ell=1}^{n} b_{ijk\ell}\, x_i x_j x_k x_\ell$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if $a_1, \ldots, a_n > 0$ and if

$$\sum_{i,j,k,\ell} b_{ijk\ell}\, x_i x_j x_k x_\ell \geq 0$$

for all x. All but two of them can be extended to treat the x^{2m} operators and their higher dimensional analogues. We note that the limit point–limit circle techniques discussed in the Appendix to Section X.1 can also be used to discuss the *one-dimensional* anharmonic oscillator.

There is one method of using Theorems X.12 and X.14 (the Kato–Rellich and Wüst theorems) in tandem to treat operators which are not directly amenable to perturbation theorems. The method, known as Konrady's trick, will provide our first proof that the anharmonic oscillator Hamiltonian is essentially self-adjoint on $C_0^\infty(\mathbb{R})$. Konrady's trick proves that $X + Y$ is essentially self-adjoint on some set D by a three-step process which is schematically of the following form:

(a) One finds some Z so that $X + Z$ is essentially self-adjoint on $D \subset D(X) \cap D(Z)$. Z is not a small perturbation of X. A typical example is to take Z to be a power of X and $D = C^\infty(X)$.

(b) One proves $X + Z + Y$ is essentially self-adjoint on D. Typically, this is done by proving Y is $(X + Z)$-bounded with bound less than one, so that the Kato–Rellich theorem is applicable. Notice that since Z is not a small perturbation of X, Y can be $(X + Z)$-bounded even if it is not X-bounded.

(c) One proves an estimate $\|Z\psi\| \leq \|(X + Y + Z)\psi\| + b\|\psi\|$ for some b and all $\psi \in D$. By Wüst's theorem, $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D. Typically one proves this estimate (which is of the form (X.21a)) by proving the stronger estimate on operators (of the form of (X.21c)): $Z^2 \leq (X + Y + Z)^2 + b^2$.

Of course, to apply Konrady's trick, one must choose Z cleverly.

Example 6 (essential self-adjointness of $-d^2/dx^2 + x^2 + x^4$ on $C_0^\infty(\mathbb{R})$; first proof) Let $X = -d^2/dx^2 + x^2$ and $Y = x^4$. Let $Z = cX^2$ where c is a positive constant which we will choose later in the proof. Let $D = C^\infty(X) = \mathscr{S}(\mathbb{R})$. We will prove essential self-adjointness of $X + Y$ on D; the simple argument that allows one to conclude essential self-adjointness on $C_0^\infty(\mathbb{R})$ from this is left to the reader. We know that the Hermite functions (see the Appendix to Section V.3) are a complete orthonormal set for $L^2(-\infty, \infty)$ (Chapter IX, Problems 6 and 7), and that $X\psi_n = (2n + 1)\psi_n$. It follows from the Appendix to Section V.3, that $\mathrm{Ran}(X + 1) = \mathscr{S}(\mathbb{R})$, so we conclude that X is essentially self-adjoint on $\mathscr{S}$. By the spectral theorem, $X + Z$ is essentially self-adjoint on $D = C^\infty(X)$. This completes step (a) in Konrady's trick. In terms of the operators A, $A^\dagger$ introduced in Section V.3, $X = 2A^\dagger A + 1$, and $Y = \frac{1}{4}(A + A^\dagger)^4$. Using the inequality

$$\|A_1^\# \cdots A_n^\# \psi\| \leq c_n \|X^{n/2}\psi\| \tag{X.28}$$

(where each $A_i^\#$ is an A or an $A^\dagger$), one proves that $\|Y\psi\| \leq d\|X^2\psi\| \leq dc^{-1}\|(X + Z)\psi\|$. We thus pick $c = 2d$ and conclude that $X + Y + Z$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ by employing the Kato–Rellich theorem.

This completes step (b) of Konrady's trick. Finally, let us prove that for some constant e,

$$Z^2 \leq (X + Y + Z)^2 + e \tag{X.29}$$

We compute

$$\begin{aligned}(X + Y + Z)^2 &= (X + Y)^2 + Z^2 + Z(X + Y) + (X + Y)Z \\ &= (X + Y)^2 + Z^2 + 2cX^3 + 2cXYX + 2c[X, [X, Y]] \\ &\geq Z^2 + 2cX^3 + 2c[X, [X, Y]]\end{aligned}$$

where we have used $Y \geq 0$, and $[X, [X, Y]] = X^2Y + YX^2 - 2XYX$ together with the fact that all the manipulations we perform are legitimate when applied to vectors in $\mathscr{S}(\mathbb{R})$. Finally we note that $[X, [X, Y]]$ can be written as the sum of 16 monomials of the form $A_1^{\#}A_2^{\#}A_3^{\#}A_4^{\#}$. Thus, using Theorem X.18, (X.28), and the fact that $[X, [X, Y]]$ is symmetric, we conclude

$$-[X, [X, Y]] \leq fX^2 \leq X^3 + (f + 1)$$

This proves (X.29), and thereby, applying Wüst's theorem, we conclude that $X + Y = X + Y + Z - Z$ is essentially self-adjoint on D.

We will use Konrady's trick again in Example 3 of Section X.9. (See also Problem 22.)

X.3 Positivity and self-adjointness I: Quadratic forms

We have already proven several results about positive or semibounded operators; see, for example, Theorems X.12 and X.17. In this section and the next, we exploit two different notions of positivity to prove a variety of self-adjointness theorems. In this section we use the concept of positive operator and quadratic form techniques. In the next, we use the fact that if a Hilbert space is of the form $L^2(M, d\mu)$, which is usual in applications, then it contains the distinguished cone of functions that are nonnegative a.e. Further applications of positivity conditions appear throughout this chapter, for example in Theorem X.55, and in later chapters, for example, in Section XIII.11.

It follows from the first corollary to Theorem X.1 that a semibounded symmetric operator A has equal deficiency indices, and therefore by von

Neumann's theorem, such an operator always has self-adjoint extensions. There is a distinguished extension, called the **Friedrichs extension**, which is obtained from the quadratic form associated to A.

Theorem X.23 (the Friedrichs extension) Let A be a positive symmetric operator and let $q(\varphi, \psi) = (\varphi, A\psi)$ for $\varphi, \psi \in D(A)$. Then q is a closable quadratic form and its closure $\hat{q}$ is the quadratic form of a unique self-adjoint operator $\hat{A}$. $\hat{A}$ is a positive extension of A, and the lower bound of its spectrum is the lower bound of q. Further, $\hat{A}$ is the only self-adjoint extension of A whose domain is contained in the form domain of $\hat{q}$.

Proof Let $(\varphi, \psi)_{+1} = q(\varphi, \psi) + (\varphi, \psi)$. Then $(\cdot, \cdot)_{+1}$ is an inner product on $D(A)$, so we can complete $D(A)$ under $(\cdot, \cdot)_{+1}$ to obtain a Hilbert space $\mathscr{H}_{+1}$. q clearly extends to a closed form $\hat{q}$ on $\mathscr{H}_{+1}$, but to show that $\hat{q}$ is a closed form on $\mathscr{H}$, we must show that $\mathscr{H}_{+1}$ is a subset of $\mathscr{H}$. Let i: $D(A) \to \mathscr{H}$ be the identity map. Since $\|\varphi\| \leq \|\varphi\|_{+1}$, i is bounded and thus extends by the B.L.T. theorem to a bounded map $\hat{i}$: $\mathscr{H}_{+1} \to \mathscr{H}$ of norm less than or equal to one. To show that $\mathscr{H}_{+1} \subset \mathscr{H}$, we proceed to show that $\hat{i}$ is injective. Suppose that $\hat{i}(\varphi) = 0$. Then, there exist $\varphi_n \in D(A)$ so that $\|\varphi - \varphi_n\|_{+1} \to 0$ and so that $\|\hat{i}(\varphi_n)\| = \|\varphi_n\| \to 0$. Thus

$$\begin{aligned}\|\varphi\|_{+1} &= \lim_{n, m \to \infty} (\varphi_n, \varphi_m)_{+1} \\ &= \lim_{n \to \infty} \lim_{m \to \infty} \{(\varphi_m, A\varphi_n) + (\varphi_m, \varphi_n)\} \\ &= 0\end{aligned}$$

since $\varphi_n \in D(A)$ and $\|\varphi_m\| \to 0$. Thus $\hat{i}$ is injective. Notice that the proof that $\hat{i}$ is well-defined uses only the positivity of q, but the proof that $\hat{i}$ is one to one uses the hypothesis that q arises from an operator.

Since $\hat{q}$ is closed and symmetric, by Theorem VIII.15 there is a unique self-adjoint operator $\hat{A}$ so that $D(\hat{A}) \subset Q(\hat{q})$ and $\hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$ if $\varphi \in Q(\hat{q})$ and $\psi \in D(\hat{A})$. Now, suppose also that $\varphi \in D(A)$. Then by the continuity of $\hat{q}$,

$$(A\varphi, \psi) = \hat{q}(\varphi, \psi) = (\varphi, \hat{A}\psi)$$

Since, this holds for all $\psi \in D(\hat{A})$, we conclude that $\varphi \in D(\hat{A}^*) = D(\hat{A})$ and $\hat{A}^*\varphi = \hat{A}\varphi = A\varphi$. Thus $\hat{A}$ extends A. The same proof shows that if A_e is any symmetric extension of A with $D(A_e) \subset Q(\hat{q})$, then $\hat{A}$ extends A_e. Thus if A_e is self-adjoint $\hat{A} = A_e$.

The easy proof of the statement about the spectrum of A is left to the reader. ∎

In Section VIII.6 we proved that the quadratic form $q(\varphi, \psi) = \overline{\varphi(0)}\psi(0)$ on $C_0^\infty(\mathbb{R})$ is not closable. In the terminology of the above proof, the reason is that $\mathscr{H}_{+1} = \{\langle \psi, a\rangle | \psi \in L^2(\mathbb{R}), a \in \mathbb{R}\}$ where a is the "value" of ψ at zero. Thus the map i: $\langle \psi, a\rangle \to \psi$ is not 1–1.

Two nice features of the Friedrichs extensions are the preservation of the lower bound and the fact that the domain of $\hat{A}$ is contained in the form domain of $\hat{q}$. In certain cases one can say more about the domain of $\hat{A}$; see the Notes and Theorem X.32.

Example 1 Let $A = -d^2/dx^2$ on $C_0^\infty(0, 1)$. Then

$$\|\psi\|_{+1}^2 = \|d\psi/dx\|^2 + \|\psi\|^2$$

If $\psi_n \xrightarrow{\|\cdot\|_{+1}} \psi$, then ψ has an L^2 derivative. It easily follows that

$$|\psi_n(a) - \psi(a)| \to 0$$

for each $a \in [0, 1]$. Thus for all $\varphi \in D(\hat{A})$, $\varphi(0) = 0 = \varphi(1)$, i.e., the Friedrichs extension $\hat{A}$ of $-d^2/dx^2$ is the self-adjoint extension with boundary conditions $\varphi(0) = 0 = \varphi(1)$. The spectrum of this extension is $\{(n\pi)^2 | n = 1, 2, \ldots\}$ with corresponding eigenfunctions $\{\sin(n\pi x)\}$. Since $\hat{A}$ is bounded below by π, the same must be true of the original quadratic form arising from A. Thus, by an integration by parts we conclude the classical inequality

$$\int_0^1 |\varphi'(x)|^2\, dx \geq \pi^2 \int_0^1 |\varphi(x)|^2\, dx$$

for functions $\varphi \in C_0^\infty(0, 1)$. We remark that this can also be computed directly by using Fourier series. Notice that another self-adjoint extension of A may have a smaller lower bound than $\hat{A}$. For example, the self-adjoint extension with boundary conditions $\varphi'(0) = 0 = \varphi'(1)$ has lower bound zero. On the other hand, it is possible for a self-adjoint extension other than the Friedrichs extension to have the same lower bound as the Friedrichs extension. For example, the self-adjoint extension $\tilde{A}$ with boundary conditions $\varphi(0) = -\varphi(1), \varphi'(0) = -\varphi'(1)$ has eigenvalues $(n\pi)^2, n = 1, 3, \ldots$, each of multiplicity 2.

Let A_0 be the extension of A with boundary conditions $\varphi(0) = 0 = \varphi(1)$, $\varphi'(0) = -\varphi'(1)$. The reader can easily check that A_0 has deficiency indices $\langle 1, 1\rangle$. Clearly, both $\hat{A}$ and $\tilde{A}$ extend A_0. So, even in the case of deficiency indices $\langle 1, 1\rangle$, another self-adjoint extension may have the same lower bound as the Friedrichs extension.

Example 2 (weak solutions of partial differential equations) Let Ω be an open region in $\mathbb{R}^n$ and let A be the operator $-\Delta + I$ with domain $C_0^\infty(\Omega) \subset L^2(\Omega)$. A is symmetric and bounded below by one. If $\hat{A}$ is the Friedrichs extension of A, then $\hat{A} \geq I$ also, so $\mathrm{Ran}(\hat{A}) = L^2(\Omega)$. Thus, for any $g \in L^2(\Omega)$, there is an $f \in D(\hat{A})$ so that $\hat{A}g = f$. So, if $\varphi \in C_0^\infty(\Omega)$,

$$(\varphi, g) = (\varphi, \hat{A}f) = (\hat{A}\varphi, f) = ((-\Delta + I)\varphi, f)$$

That is, for each $g \in L^2(\Omega)$, the equation

$$(-\Delta + I)f = g$$

has a weak solution $f \in L^2(\Omega)$. Since $\Delta f = f - g \in L^2(\Omega)$, we can use Sobolev's lemma (Section IX.6) to show a certain amount (depending on n) of regularity for f. If $g \in C_0^\infty(\Omega)$, then applying Δ repeatedly to the equation $\Delta f = f - g$ proves that $f \in \bigcap_{m=1}^\infty W_m(\Omega)$, so in this case Sobolev's lemma implies that f is a C^∞ function.

For another application of the Friedrichs extension, see Problem 25 where the reader is asked to prove the Stieltjes moment condition, the analogue of the Hamburger condition when $[0, \infty)$ replaces $(-\infty, \infty)$. In this application, as in the above example, it is crucial that the Friedrichs extension of A has the same lower bound as A. This suggests the problem of investigating the lower bounds of the other self-adjoint extensions.

Proposition Let A be a semibounded symmetric operator with finite deficiency indices. Then any self-adjoint extension of A is bounded below (possibly with a smaller lower bound).

Proof Let $\tilde{A}$ be a self-adjoint extension of A with corresponding projection-valued measure P_Ω. Suppose that the deficiency indices of A equal n. Then by Theorem X.2, $D(\tilde{A}) = D(A) + S$ where S is an n-dimensional vector space. Let K be less than M, the lower bound of A. Then we must have $\dim P_{(K, M)} \leq n$. Otherwise we could find a vector in $D(A) \cap \mathrm{Ran}\, P_{(K, M)}$, which would contradict the fact that A is bounded below by M. Thus, $\dim P_{(-\infty, M)} \leq n$, so $\tilde{A}$ is bounded below. ∎

In the case of infinite deficiency indices, a semibounded symmetric operator can have self-adjoint extensions that are not bounded below (Problem 26). But even in this case there will always be many self-adjoint extensions that are bounded below. In fact, unless A is already essentially self-adjoint, there will be other extensions besides the Friedrichs extension which are bounded from below.

Theorem X.24 Let A be a symmetric operator that is bounded from below. If the Friedrichs extension $\hat{A}$ is the only self-adjoint extension of A that is bounded from below, then A is essentially self-adjoint.

Proof By the proposition, we need only consider the case where the deficiency indices of A equal infinity. Suppose $\hat{A}$ is the Friedrichs extension of A and let $\tilde{A}$ be a symmetric extension of A contained in $\hat{A}$ which has deficiency indices equal to one (to see how to construct such an A, consult Theorem X.2). Then A is bounded from below, so by the proposition all its self-adjoint extensions will be bounded from below. Hence A has more than one semibounded self-adjoint extension unless its deficiency indices are equal to zero. ∎

Another application of positivity and quadratic form techniques is the following theorem of von Neumann. His original operator-theoretic proof does not use quadratic forms.

Theorem X.25 Let A be a *closed* densely defined operator and let

$$D(A^*A) = \{\psi \in D(A) \,|\, A\psi \in D(A^*)\}$$

Define A^*A on $D(A^*A)$ by $(A^*A)\psi = A^*(A\psi)$. Then A^*A is self-adjoint.

Proof Define the form $b(\varphi, \psi)$ on $D(A) \times D(A)$ by $b(\varphi, \psi) = (A\varphi, A\psi)$. b is nonnegative and since A is closed as an operator, b is closed as a quadratic form. Let B be the associated self-adjoint operator given by Theorem VIII.15. We will show that $B = A^*A$. Notice that, a priori, it is not evident that there are any vectors besides the zero vector in $D(A^*A)$.

Let $\mathscr{H}_{+1} \subset \mathscr{H} \subset \mathscr{H}_{-1}$ be the scale of spaces defined by b as in the proof of Theorem VIII.15. Define $\hat{A}^*: \mathscr{H} \to \mathscr{H}_{-1}$ by $(\hat{A}^*\varphi)(\psi) = (\varphi, A\psi)$. By the definition of adjoint $D(A^*) = \{\varphi \,|\, \hat{A}^*\varphi \in \mathscr{H}\}$ and $A^* = \hat{A}^* \restriction D(A^*)$. Let $\hat{B}: \mathscr{H}_{+1} \to \mathscr{H}_{-1}$ be the natural map given by $(\hat{B}\varphi, \psi) = b(\varphi, \psi)$. From the proof of Theorem VIII.15, we have that $D(B) = \{\varphi \in \mathscr{H}_{+1} \,|\, \hat{B}\varphi \in \mathscr{H}\}$ and $B = \hat{B} \restriction D(B)$. Now, suppose $\varphi, \psi \in \mathscr{H}_{+1}$. Then

$$[\hat{A}^*(A\varphi)](\psi) = (A\varphi, A\psi) = (\hat{B}\varphi)(\psi)$$

so $\hat{B} = \hat{A}^*A$. Thus

$$\begin{aligned} D(B) &= \{\varphi \in \mathscr{H}_{+1} \,|\, \hat{B}\varphi \in \mathscr{H}\} \\ &= \{\varphi \in \mathscr{H}_{+1} \,|\, A^*(A\varphi) \in \mathscr{H}\} \\ &= \{\varphi \in \mathscr{H}_{+1} \,|\, A\varphi \in D(A^*)\} \\ &= D(A^*A) \end{aligned}$$

and $B = \hat{B} \restriction D(B) = A^*A$. ∎

The proof has the following corollary.

Corollary Let A be a closed operator. Then any core for A is a form core for A^*A.

Corollary If A is symmetric and A^2 is densely defined, then A^*A is the Friedrichs extension of A^2.

Example 3 Let $A = i\, d/dx$ with domain

$$D(A) = \{\varphi \,|\, \varphi \in AC[0, 1], \varphi(0) = \varphi(1) = 0\}$$

We have already computed that

$$D(A^*) = \{\varphi \,|\, \varphi \in AC[0, 1]\}$$

and $A^*\varphi = i\, d\varphi/dx$. It follows immediately from the definitions of $D(AA^*)$ and $D(A^*A)$ and the above theorem that A^*A is the self-adjoint extension of $-d^2/dx^2$ with boundary conditions $\varphi(0) = 0 = \varphi(1)$, and AA^* is the self-adjoint extension of $-d^2/dx^2$ with boundary conditions $\varphi'(0) = 0 = \varphi'(1)$.

Example 4 (Schrödinger operators with magnetic fields) One can use quadratic form methods to define self-adjoint Hamiltonians of the form of (X.26) although not with explicit control over operator domains. Consider first the case $V = 0$. Suppose that $\mathbf{A} \in L^2(\mathbb{R}^3)_{\text{loc}}$. Let T_j denote the closure of the symmetric operator $-i^{-1}\, \partial/\partial x_j + eA_j/c$ on $C_0^\infty(\mathbb{R}^3)$. A simple extension of Theorem X.25 shows that $H = \sum_{i=1}^3 T_i^*T_i$ can be defined as a self-adjoint operator on

$$\left\{\psi \in \bigcap_{i=1}^3 D(T_i) \,\middle|\, T_i\psi \in D(T_i^*)\right\}$$

The same method works if $V \geq 0$ with $V \in L^1_{\text{loc}}$. In either case one has

$$Q(H) = \left(\bigcap_{i=1}^3 D(T_i)\right) \cap Q(V)$$

In the next section we will describe $D(-\Delta + V)$ when $V \geq 0$ and $V \in L^1_{\text{loc}}$.

We conclude this section by summarizing in one place some of the facts which we have proven about strictly positive symmetric operators. Of course every semibounded symmetric operator becomes strictly positive after translation by a constant.

Theorem X.26 Let A be a strictly positive symmetric operator, i.e. $(A\varphi, \varphi) \geq c(\varphi, \varphi)$ for all $\varphi \in D(A)$ and some $c > 0$. Then the following are equivalent:

(a) A is essentially self-adjoint.
(b) $\mathrm{Ran}(A)$ is dense.
(c) $\mathrm{Ker}(A^*) = \{0\}$.
(d) A has only one semibounded self-adjoint extension.

X.4 Positivity and self-adjointness II: Pointwise positivity

The results of the previous section depended on exploiting the notion of positive operator, something which makes sense on any Hilbert space $\mathscr{H}$. In this section, we exploit a different type of positivity associated with L^2 spaces—that of a vector being positive. This is not a notion intrinsic to $\mathscr{H}$ alone but to its realization as an L^2 space. This notion will appear again from time to time and will play a major role in Section XIII.11. Since the Hilbert space of quantum mechanics is typically given as an L^2 space, there is present in such cases the structure associated with positive vectors. Given the positive vectors, there is an associated notion of positive multiplication operator, i.e., a multiplication operator $\psi(x) \mapsto V(x)\psi(x)$ which takes the positive vectors into themselves. The major results in this section concern the essential self-adjointness of $-\Delta + V$ if $V \geq 0$ under very weak additional assumptions, and of magnetic field Schrödinger Hamiltonians in a general situation.

First, we extend the notion of positivity to distributions:

Definition Let $T \in \mathscr{D}'(\mathbb{R}^n)$. We say that T is **positive** and write $T \geq 0$ if and only if $T(f) \geq 0$ whenever $f \in \mathscr{D}$ is pointwise nonnegative. If $T, S \in \mathscr{D}$ and $T - S \geq 0$, we write $T \geq S$.

We immediately note two facts about positive distributions. First, if $T(f) = \int F(x) f(x)\, d^n x$ where F is a continuous function on $\mathbb{R}^n$, then $T \geq 0$ if and only if $F(x) \geq 0$ for all x. Secondly, if T_n is a sequence of positive distributions and $T_n \to T$ weakly, then T is positive.

Our self-adjointness result depends on the following elegant distributional inequality:

Theorem X.27 (Kato's inequality) Let u be a locally L^1 function on $\mathbb{R}^n$ whose distributional Laplacian Δu is also a locally L^1 function. Define

$$(\mathrm{sgn}\, u)(x) = \begin{cases} 0 & \text{if } u(x) = 0 \\ \overline{u(x)}/|u(x)| & \text{if } u(x) \neq 0 \end{cases}$$

so that $\mathrm{sgn}\, u$ is L^∞ and $(\mathrm{sgn}\, u)\, \Delta u$ is a locally L^1 function and hence a distribution. Then the distributional Laplacian $\Delta |u|$ of $|u|$ obeys the following distributional inequality:

$$\Delta |u| \geq \mathrm{Re}[(\mathrm{sgn}\, u)\, \Delta u] \tag{X.30}$$

Example 1 To help understand this result, consider the case $n = 1$ where $u \in C^\infty(\mathbb{R})$ is strictly positive if $x > 0$ and strictly negative if $x < 0$. Then $|u|$ is C^∞ on $\mathbb{R}\backslash\{0\}$, but at $x = 0$ its first derivative has a discontinuity of magnitude $2u'(0)$. Thus

$$\frac{d^2}{dx^2} |u| = (\mathrm{sgn}\, u) \frac{d^2}{dx^2} u + 2u'(0)\, \delta(x)$$

so we can see (X.30) explicitly since $u'(0) \geq 0$.

Proof of Theorem X.27 Suppose first that u is C^∞ and let u_ε be given by

$$u_\varepsilon(x) = \sqrt{|u(x)|^2 + \varepsilon^2} \tag{X.31}$$

so that u_ε is C^∞. Differentiating the square of (X.31),

$$2u_\varepsilon(x)[\mathrm{grad}\, u_\varepsilon(x)] = 2\, \mathrm{Re}[\overline{u(x)}(\mathrm{grad}\, u(x))] \tag{X.32}$$

Since (X.31) implies that $|u_\varepsilon| \geq |u|$, (X.32) implies that

$$|\mathrm{grad}\, u_\varepsilon| \leq |\overline{u(x)}|\, |u_\varepsilon(x)|^{-1} |\mathrm{grad}\, u(x)| \leq |\mathrm{grad}\, u(x)| \tag{X.33}$$

Taking the divergence of (X.32) we see that

$$u_\varepsilon\, \Delta u_\varepsilon + |\mathrm{grad}\, u_\varepsilon|^2 = \mathrm{Re}(\bar{u}\, \Delta u) + |\mathrm{grad}\, u|^2$$

so on account of (X.33)

$$u_\varepsilon\, \Delta u_\varepsilon \geq \mathrm{Re}(\bar{u}\, \Delta u)$$

pointwise and thus in distributional sense.

As a result,

$$\Delta u_\varepsilon \geq \mathrm{Re}(\mathrm{sgn}_\varepsilon(u)\, \Delta u) \tag{X.34}$$

where

$$\mathrm{sgn}_\varepsilon(u(x)) = \overline{u(x)}/u_\varepsilon(x)$$

Now let u be an arbitrary locally L^1 function with $\Delta u \in L^1_{\text{loc}}$ and let j_δ be an approximate identity, i.e., let $j_\delta(x) = j(x/\delta)\delta^{-n}$ where $j \geq 0$, $j \in C_0^\infty(\mathbb{R}^n)$ and $\int j(x)\, d^n x = 1$. Let $u^\delta = u * j_\delta$. Since u^δ is C^∞,

$$\Delta(u^\delta)_\varepsilon \geq \operatorname{Re}(\operatorname{sgn}_\varepsilon(u^\delta)\, \Delta u^\delta) \tag{X.35}$$

for each ε, $\delta > 0$. Fix $\varepsilon > 0$ and take $\delta \to 0$. Then $u^\delta \to u$ in local L^1 norm and thus also in $\mathscr{D}'$. In particular, by passing to a subsequence, we can suppose that $u^\delta(x) \to u(x)$ pointwise a.e. Thus $\operatorname{sgn}_\varepsilon(u^\delta) \to \operatorname{sgn}_\varepsilon(u)$ pointwise a.e. Since $\Delta u^\delta = (\Delta u)^\delta$ and Δu is also in L^1_{loc}, $\Delta u^\delta \to \Delta u$ in L^1_{loc}. It is now easy to see that $\operatorname{sgn}_\varepsilon(u^\delta)\, \Delta u^\delta \to \operatorname{sgn}_\varepsilon(u)\, \Delta u$ in $\mathscr{D}'$, so taking $\delta \to 0$ in (X.35) we conclude that (X.34) holds for u. Now take $\varepsilon \to 0$. Then $\operatorname{sgn}_\varepsilon(u) \to \operatorname{sgn}(u)$ pointwise with a uniform bound ($|\operatorname{sgn}_\varepsilon u| \leq 1$), so that the two sides of (X.34) converge in $\mathscr{D}'$ to the two sides of (X.30). ∎

Typical of the applications of Theorem X.27 is

Theorem X.28 Let $V \in L^2(\mathbb{R}^n)_{\text{loc}}$ with $V \geq 0$ pointwise. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof By Theorem X.26, we need only show that

$$(-\Delta + V + 1)^* u = 0 \tag{X.36}$$

implies that $u = 0$. But by the fact that $-\Delta + V$ is given with domain C_0^∞, (X.36) is equivalent to

$$(-\Delta + V + 1)u = 0, \qquad u \in L^2(\mathbb{R}^n) \tag{X.37}$$

where the derivative in question is a distributional derivative. (X.35) implies that $\Delta u = Vu + u$ is in L^1_{loc} since u and $V + 1$ are in L^2_{loc}. Thus, by Theorem X.27

$$\Delta|u| \geq \operatorname{Re}(\operatorname{sgn} u\, \Delta u) = \operatorname{Re}(\operatorname{sgn} u\, (Vu + u)) = (V + 1)|u| \tag{X.38}$$

In particular, $\Delta|u| \geq 0$.

Let j_δ be an approximate identity, as in the previous theorem, and let $w = |u|$, $w^\delta = w * j^\delta$. Then $\Delta w^\delta = w * \Delta j_\delta \in L^2$, so w^δ is in $D(\Delta)$ and thus $(w^\delta, \Delta w^\delta) \leq 0$ with equality only if $w^\delta = 0$. But $\Delta w^\delta = \Delta|u| * j_\delta \geq 0$ in distributional sense and so $\Delta w_\delta \geq 0$ pointwise. Thus, $(w^\delta, \Delta w^\delta) \geq 0$ so $w^\delta = 0$. Since $w^\delta \to w$ as $\delta \to 0$, $w = 0$ and therefore $u = 0$. ∎

Example 2 (essential self-adjointness of $-d^2/dx^2 + x^2 + x^4$ on $C_0^\infty(\mathbb{R})$; second proof) Since $x^2 + x^4$ is positive, and locally L^2, Theorem X.28 implies that $-d^2/dx^2 + x^2 + x^4$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$. More generally, $-\Delta + P(x_1, \ldots, x_n)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ for any polynomial bounded from below.

Example 3 Let $V(x) = 2|x|^{-2}$ on $L^2(\mathbb{R}^5)$. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$ by Theorem X.28 (or by Theorem X.11). On the other hand, $V \in L^2_{\text{loc}}$ and $-\Delta - V$ is bounded below but not essentially self-adjoint on $C_0^\infty(\mathbb{R}^5)$ (see Theorem X.11 and Example 4 in Section X.2). Thus the condition $V \geq 0$ in Theorem X.28 cannot be completely eliminated.

Theorem X.28 can be extended in a variety of ways.

Theorem X.29 Let $V = V_1 + V_2$ where $V_1 \geq 0$, $V_1 \in L^2(\mathbb{R}^n)_{\text{loc}}$ and where V_2 is a $-\Delta$-bounded multiplication operator with relative bound $a < 1$. Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. In particular, if V is a multiplication operator with $V_+ = \max(V, 0) \in L^2_{\text{loc}}$ and $V_- = \min(V, 0) \in L^p + L^\infty$ where $p = 2$ if $n \leq 3$, $p > 2$ if $n = 4$ and $p = n/2$ if $n \geq 5$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof By following the arguments in Theorem X.28, we need only show that $(-\Delta + V + b)u = 0$ (distributional sense) and $u \in L^2(\mathbb{R}^n)$ implies that $u = 0$, where b is some large constant to be chosen below. Since $C_0^\infty(\mathbb{R}^n) \subset D(-\Delta) \subset D(V_2)$, V_2 is in L^2_{loc}; so by using Kato's inequality, we obtain the analogue of (X.38)

$$\Delta|u| \geq (V + b)|u| \geq (V_2 + b)|u|$$

Thus

$$(-\Delta + b)|u| \leq -V_2|u| \tag{X.39}$$

Now, by the explicit form of its kernel (Problem 50 of Chapter IX), $(-\Delta + b)^{-1}$ takes positive elements of $\mathscr{S}(\mathbb{R}^n)$ into other positive elements; and so, since it is self-adjoint, positive elements of $\mathscr{S}'(\mathbb{R}^n)$ into other positive tempered distributions. Moreover, since V_2 is $-\Delta$-bounded

$$\left| \int V_2(x)|u(x)|f(x)\, dx \right| \leq (\text{const})\|u\|_{L^2}\|(-\Delta + 1)f\|$$

so $V_2|u|$ is a tempered distribution. Thus by (X.39),

$$|u| \leq -(-\Delta + b)^{-1} V_2|u| \tag{X.40}$$

Since V_2 has $-\Delta$ bound $a < 1$, we can choose b so that $\|(-\Delta + b)^{-1}V_2\| \leq \frac{1}{2}(a + 1) < 1$. Then by (X.40)

$$\|u\| \leq \|(-\Delta + b)^{-1}V_2\| \, \|u\|$$

so $\|u\| = 0$. ∎

We state without proof the following theorem which generalizes part of Theorem X.11 to the noncentral case:

Theorem X.30 (Kalf–Walter–Schmincke–Simon theorem) Let $V = V_1 + V_2$ with $V_2 \in L^\infty(\mathbb{R}^n)$ and $V_1 \in L^2(\mathbb{R}^n\backslash\{0\})_{\text{loc}}$ obeying

$$V_1(\mathbf{r}) \geq -n(n-4)/4r^2$$

Then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$.

References to the proof which exploits Kato's inequality can be found in the Notes.

There is another proof of Theorem X.29 which is of interest because it exploits the following very beautiful result about positivity in L^2 spaces:

Definition A bounded operator A on $L^2(X, d\mu)$ is called **positivity preserving** if $(A\varphi)(x) \geq 0$ a.e. whenever $\varphi(x) \geq 0$ a.e. A semigroup $T(t)$ is called positivity preserving if it is positivity preserving for each $t \geq 0$.

Theorem X.31 (the Davies–Faris theorem) Let H_0 be a positive self-adjoint operator on $L^2(X, d\mu)$ such that e^{-tH_0} is positively preserving. Let V be a multiplication operator with $V \geq 0$. Suppose that $H = H_0 + V$ is essentially self-adjoint on $D(H_0) \cap D(V)$. Let W be an H_0-bounded multiplication operator. Then W is H-bounded. In fact, if

$$\|W\psi\| \leq a\|(H_0 + b)\psi\| \qquad \text{all} \quad \psi \in D(H_0)$$

then

$$\|W\psi\| \leq a\|(H + b)\psi\| \qquad \text{all} \quad \psi \in D(H)$$

Proof Suppose that $\|W(H_0 + b)^{-1}\| \leq a$. We will show that

$$\|W(H + b)^{-1}\| \leq a$$

Since e^{-tH_0} is positivity preserving, so is $(H_0 + b)^{-1} = \int_0^\infty e^{-bt}e^{-tH_0}\,dt$. Also, by the Trotter product formula, $e^{-tH} = s - \lim_{n\to\infty}(e^{-tH_0/n}e^{-tV/n})^n$ is positivity preserving, and, so by the same argument, $(H + b)^{-1}$ is positivity preserving. We will prove later (see Theorem X.55) that if A is bounded and positivity preserving, then $|A\psi| \leq A|\psi|$ pointwise for all ψ. Thus we need only prove that

$$\|W(H + b)^{-1}|\psi|\| \leq a\|\psi\|$$

for all ψ. If we can show that (pointwise)

$$0 \leq (H + b)^{-1}\varphi \leq (H_0 + b)^{-1}\varphi \tag{X.41a}$$

for all $\varphi \geq 0$, it follows that (pointwise)

$$0 \leq |W|(H + b)^{-1}\varphi \leq |W|(H_0 + b)^{-1}\varphi \tag{X.41b}$$

and

$$\|W(H + b)^{-1}|\psi|\| \leq a\|\psi\|$$

for all ψ.

So suppose that $\varphi \geq 0$. Then, since $|e^{-sV}| \leq 1$ and e^{-sH_0} is positivity preserving,

$$e^{-sH_0}(1 - e^{-sV})\varphi \geq 0$$

so

$$0 \leq (e^{-sH_0}e^{-sV})\varphi \leq e^{-sH_0}\varphi \tag{X.42}$$

Iterating (X.42), we get

$$0 \leq (e^{-t/nH_0}e^{-t/nV})^n\varphi \leq e^{-tH_0}\varphi$$

So by the Trotter product formula

$$0 \leq e^{-tH}\varphi \leq e^{-tH_0}\varphi \tag{X.43}$$

(X.41b) follows from (X.43) by the Laplace transform formula for $(H + b)^{-1}$ in terms of e^{-tH}. ∎

As a corollary of the Davies–Faris theorem we have:

Second Proof of Theorem X.29 By Theorem X.28, $-\Delta + V_1$ is essentially self-adjoint on $D(\Delta) \cap D(V_1)$. Moreover, $e^{t\Delta}$ is positivity preserving on account of its explicit kernel (IX.31). Thus, by hypothesis, and Theorem X.31, V_2 is $-\Delta + V_1$ bounded with bound less than 1, so $-\Delta + V_1 + V_2$ is essentially self-adjoint on any core for $-\Delta + V_1$ by the Kato–Rellich theorem. ∎

Kato's inequality can also be used to study $D(-\Delta + V)$ when $-\Delta + V$ is defined as a sum of quadratic forms:

Theorem X.32 Let $V \geq 0$ be in $L^1_{\text{loc}}(\mathbb{R}^n)$. Let $H = -\Delta + V$ defined as a sum of quadratic forms. Then $D(H)$ equals

$$\{\varphi \in L^2(\mathbb{R}^n) \,|\, V\varphi \in L^1_{\text{loc}}\,;\, (-\Delta\varphi + V\varphi)_{\text{dist}} \in L^2\} \tag{X.44}$$

where $(-\Delta\varphi + V\varphi)_{\text{dist}}$ means the distribution $f \to \int \varphi(-\Delta f) + \int (V\varphi)f$. Moreover, $H\varphi = (-\Delta\varphi + V\varphi)_{\text{dist}}$.

Proof Let T be the operator with domain (X.44) and $T\varphi = -\Delta\varphi + V\varphi$. We first claim that T extends H. For let $\varphi \in D(H) \subset Q(H) = Q(-\Delta) \cap Q(V)$. Since $\varphi \in Q(V)$ we have $|V|^{1/2}\varphi \in L^2$ and since $|V|^{1/2} \in L^2_{\text{loc}}$, we conclude that $V\varphi \in L^1_{\text{loc}}$. Moreover $H\colon \mathscr{H}_{+1} \to \mathscr{H}_{-1}$ is $-\Delta + V$ defined in the distributional sense, so by the construction of $D(H)$ in Theorem VIII.15, $H\varphi = -\Delta\varphi + V\varphi \in L^2$, i.e., $\varphi \in D(T)$ and $H\varphi = T\varphi$.

Suppose now that $\eta \in D(T)$. Since H is self-adjoint and positive, we can find $\varphi \in D(H)$ with $(T + 1)\eta = (H + 1)\varphi$. Let $\psi = \eta - \varphi$. Then, since T extends H, $(T + 1)\psi = 0$. Since $\psi \in D(T)$ we have that $-\Delta\psi = T\psi - V\psi = -\psi - V\psi \in L^1_{\text{loc}}$, so Kato's inequality is applicable and assures us that

$$\Delta|\psi| \geq (\operatorname{sgn}\psi)(\psi + V\psi) = (V + 1)|\psi| \geq 0$$

As in the proof of Theorem X.28, this implies that $\psi = 0$. Thus $\eta = \varphi \in D(H)$, i.e., $D(T) \subset D(H)$. So $T = H$. ∎

Next, we turn to the application of Kato's inequality to Schrödinger operators with magnetic fields. We first need a more general version of the inequality:

Theorem X.33 Let a_k $(k = 1, \ldots, n)$ be real-valued functions in $C^1(\mathbb{R}^n)$. Let D_k be the operator on $\mathscr{D}'$

$$D_k T = \frac{1}{i}\frac{\partial T}{\partial x_k} - a_k T$$

and let $D^2 = \sum D_k^2$. Then, for any u with $u \in L^1_{\text{loc}}$ and $D^2u \in L^2_{\text{loc}}$,

$$\Delta|u| \geq -\operatorname{Re}[(\operatorname{sgn} u)D^2u] \tag{X.45}$$

The main additional idea needed to prove Theorem X.33, given the proof of Theorem X.27, is:

Lemma Under the hypotheses of Theorem X.33, Δu and ∇u are in L^1_{loc}.

Proof We need only show that Δu, ∇u are locally L^1 near $x = 0$. Let f be a function in C_0^∞, identically 1 near 0. Then by explicit computation

$$(-\Delta + 1)(fu) = h_1 + \nabla \cdot \mathbf{h}_2 \tag{X.46}$$

with

$$h_1 = fD^2u + (\Delta f)u + if(\nabla \cdot \mathbf{a})u - 2i(\nabla f) \cdot \mathbf{a}u + (a^2 + 1)fu$$
$$\mathbf{h}_2 = 2if\mathbf{a}u - 2(\nabla f)u$$

What is important is that by hypothesis, $h_1 \in L^1$, $\mathbf{h}_2 \in L^2$, and $fu \in L^2$. Thus, all the functions in (X.46) lie in $\mathscr{S}'(\mathbb{R}^n)$. Since $(-\Delta + 1)$ is invertible on $\mathscr{S}$, it is invertible on $\mathscr{S}'$, so that

$$fu = (-\Delta + 1)^{-1}h_1 + (-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2$$

and

$$\nabla(fu) = \nabla(-\Delta + 1)^{-1}h_1 + \nabla(-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2$$

Now, since $\mathbf{h}_2 \in L^2$, its Fourier transform is in L^2 so that

$$\nabla_i(-\Delta + 1)^{-1}\nabla \cdot \mathbf{h}_2 = \mathscr{F}^{-1}\left(p_i(p^2 + 1)^{-1}\sum_j p_j \cdot \hat{h}_j\right)$$

is in L^2 since $p_i p_j(p^2 + 1)^{-1} \in L^\infty$. Let $G_i(x)$ be the distribution with $\hat{G}_i(p) = (2\pi)^{-n/2}p_i(p^2 + 1)^{-1}$. By following the methods of Problem 50 of Chapter IX, $G_i(x)$ is continuous away from $x = 0$, falling exponentially at infinity and $|G_i(x)| \leq C|x|^{-n+1}$ ($\ln|x|$ if $n = 1$). Thus $G_i \in L^p$ for some $p > 1$ and therefore $G_i * h_1 \in L^p$ by Young's inequality. We conclude that $\nabla(fu)$ lies in L^1_{loc} and so ∇u is L^1_{loc} near 0. Now, since $\nabla u \in L^1_{\text{loc}}$, we conclude that $\nabla \cdot \mathbf{h}_2 \in L^1_{\text{loc}}$ so by (X.46), $-\Delta u \in L^1_{\text{loc}}$. ∎

Proof of Theorem X.33 Suppose first that $u \in C^\infty(\mathbb{R}^n)$ and let u_ε be given by (X.31). Then since $\operatorname{Im}(\overline{u(x)}a_j(x)u(x)) = 0$, (X.32) implies that

$$u_\varepsilon \operatorname{grad}_k u_\varepsilon = \operatorname{Re}[\overline{u(x)}(iD_k u)(x)] \tag{X.47}$$

so that

$$|\operatorname{grad} u_\varepsilon| \leq |Du| \tag{X.48}$$

Taking the divergence of (X.47) and using

$$\begin{aligned}\partial_k[\bar{u}(iD_k u)] &= (\partial_k \bar{u})(iD_k u) + \bar{u}(\partial_k(iD_k u)) \\ &= \overline{[(\partial_k - ia_k)u]}(iD_k u) + \bar{u}(\partial_k - ia_k)(iD_k u) \\ &= |D_k u|^2 - \bar{u}D_k^2 u\end{aligned}$$

we see that

$$\Delta u_\varepsilon \geq -\mathrm{Re}[\mathrm{sgn}_\varepsilon(u) D^2 u] \tag{X.49}$$

We have used (X.48) as in the proof of Theorem X.27. As in that proof, we now approximate a given $u \in L^2_{\mathrm{loc}}$ with $D^2u \in L^1_{\mathrm{loc}}$ by u^δ's. Since, by the lemma, $u \in L^2_{\mathrm{loc}}$ and $D^2u \in L^1_{\mathrm{loc}}$ imply that Δu and $\nabla u \in L^1_{\mathrm{loc}}$, we conclude that $D^2u^\delta \to D^2u$ in L^1_{loc}. Thus (X.49) holds for any u obeying the hypothesis of the theorem. (X.45) follows from (X.49) by letting ε approach 0. ∎

Theorem X.34 Let $a_k \in C^1(\mathbb{R}^n)$. Let $V = V_1 + V_2$ with V_1, V_2 obeying the hypotheses of Theorem X.29. Then

$$H = -\sum_{j=1}^{n} \frac{1}{2m_j}(\partial_j - ia_j)^2 + V$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof One just follows the proof of Theorem X.29 using (X.45) in place of (X.30), noting that the u to which we want to apply (X.45) is in L^2_{loc} and not merely in L^1_{loc}. ∎

Example 4 (the Zeeman effect) Let $\mathbf{a}(\mathbf{x}) = \frac{1}{2}\mathbf{x} \times \mathbf{B}_0$ where $\mathbf{B}_0$ is constant. The Hamiltonian of an N-electron atom in a constant external magnetic field is

$$H = -\frac{1}{2M}(\partial_0 - iNe\mathbf{a}(\mathbf{x}_0)/c)^2 - \frac{1}{2m}\sum_{n=1}^{N}(\partial_n + ie\mathbf{a}(\mathbf{x}_n)/c)^2$$
$$-\sum_{n=1}^{N}\frac{Ne^2}{|\mathbf{x}_n - \mathbf{x}_0|} + \frac{1}{2}\sum_{n\neq m}\frac{e^2}{|\mathbf{x}_n - \mathbf{x}_m|}$$

By Theorem X.34, H is essentially self-adjoint of $C_0^\infty(\mathbb{R}^{3N+3})$.

One can considerably weaken the smoothness hypotheses on $\mathbf{a}$ if one imposes the **Coulomb gauge condition**, $\mathrm{div}\,\mathbf{a} = 0$ (distributional sense). Notice in that case

$$D^2u = -\Delta u - 2i\mathbf{a}\cdot\nabla u + \mathbf{a}^2 u$$

so that one can define D^2 on C_0^∞ without any smoothness hypothesis on $\mathbf{a}$; only $a \in L^4_{\mathrm{loc}}$ is needed. The extra condition $\mathrm{div}\,\mathbf{a} = 0$ is quite common in the physics literature. To explain why, let us proceed formally. Given

$\lambda(x)$, let $\tilde{\mathbf{a}} = \mathbf{a} + \mathrm{grad}\,\lambda$. Notice that this does not change the magnetic field $\mathbf{B} = \mathrm{curl}\,\mathbf{a}$, i.e., $\mathrm{curl}\,\mathbf{a} = \mathrm{curl}\,\tilde{\mathbf{a}}$. If $\tilde{\mathbf{D}} = (i\partial - \tilde{\mathbf{a}})$, then

$$\tilde{\mathbf{D}} = e^{-i\lambda}\mathbf{D}e^{+i\lambda}$$

so that

$$e^{-i\lambda}(-D^2 + V)e^{+i\lambda} = -\tilde{D}^2 + V$$

Thus $-D^2 + V$ and $-\tilde{D}^2 + V$ are formally unitarily equivalent and the gauge transformation $\mathbf{a} \mapsto \tilde{\mathbf{a}}$ does not change the magnetic field. If λ is not C^∞, $-\tilde{D}^2 + V$ may have $C_0^\infty(\mathbb{R}^3)$ for a core, while it is not a core for $-D^2 + V$ (rather $e^{+i\lambda}(C_0^\infty)$ will be a core). Thus as regards essential self-adjointness on $C_0^\infty(\mathbb{R}^3)$, one must be prepared to change to a convenient gauge. By solving the partial differential equation $-\Delta\lambda = \mathrm{div}\,\mathbf{a}$, we can always find $\tilde{\mathbf{a}}$ with $\mathrm{div}\,\tilde{\mathbf{a}} = 0$ so that $\mathbf{a}$ and $\tilde{\mathbf{a}}$ are related by a gauge transformation.

The following theorem is proven in a reference to be found in the Notes.

Theorem X.35 Let V obey the conditions of Theorem X.29. Suppose that $\tilde{\mathbf{a}} \in L^q_{\mathrm{loc}}(\mathbb{R}^n)$ with $q \geq 4$, $q > n$, and with $\mathrm{div}\,\tilde{\mathbf{a}} = 0$ (distributional sense). Then

$$-\sum_{j=1}^{n}(\partial_j - ia_j)^2 + V$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

X.5 The commutator theorem

Many of the self-adjointness techniques that we have discussed so far apply only to semibounded operators or forms. Further, the Kato–Rellich and KLMN theorems have the feature that perturbations of positive operators are semibounded. In this section we prove several theorems which are useful for proving the self-adjointness of nonsemibounded operators. At the end of the section we apply the theorem to the Stark effect Hamiltonian, i.e., the Hamiltonian of an atom in a constant electric field.

Although the operator A whose self-adjointness we wish to establish will not be semibounded, we will assume that A can be estimated in various ways by an auxiliary self-adjoint operator N that is semibounded.

Throughout this section we will assume that $N \geq I$. We will denote by $\mathscr{H}_n$, $n = 0, \pm 1, \pm 2, \ldots$, the completion of $D(N^{n/2})$ in the norm

$$\|\psi\|_n = \|N^{n/2}\psi\| \tag{X.50}$$

We thus have the scale of spaces $\cdots \mathscr{H}_n \supset \mathscr{H}_{n+1} \cdots$ discussed in the Appendix to Section IX.4 and introduced for the cases $n = 0, \pm 1$ in Section VIII.6. Recall that for $n > 0$, $\mathscr{H}_n = D(N^{n/2})$ and that $\mathscr{H}_{-n}$ can be identified with $\mathscr{H}_n^*$.

Suppose that $a(\cdot, \cdot)$ is a quadratic form on $Q(a) = D(N^{n/2})$ which satisfies

$$|a(\varphi, \psi)| \leq c\|\varphi\|_n \|\psi\|_n \tag{X.51}$$

Thus for each $\varphi \in \mathscr{H}_n$, there is a $\tilde{\varphi} \in \mathscr{H}_{-n}$ so that $a(\varphi, \psi) = \tilde{\varphi}(\psi)$ for all $\psi \in \mathscr{H}_n$. The map $\varphi \overset{A}{\mapsto} \tilde{\varphi}$ is linear and bounded so $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$. Conversely, any $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ gives rise to a quadratic form $a(\cdot, \cdot)$ on $Q(a) = D(N^{n/2})$ satisfying (X.51). For such an A, the adjoint A^* is a bounded operator from $\mathscr{H}_{-n}^*$ to $\mathscr{H}_n^*$. But since $\mathscr{H}_{-n}^*$ and $\mathscr{H}_n^*$ are naturally isomorphic to $\mathscr{H}_n$ and $\mathscr{H}_{-n}$, A^* is in a natural way also a bounded operator from $\mathscr{H}_n$ to $\mathscr{H}_{-n}$. If $A = A^*$, then we say that $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ is **symmetric**. Clearly, this is equivalent to saying that the corresponding form $a(\cdot, \cdot)$ is symmetric.

Given an $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$ we can define $[N, A]$ as an operator from $\mathscr{H}_{n+2}$ to $\mathscr{H}_{-n-2}$ by

$$[N, A]\psi = N(A\psi) - A(N\psi), \qquad \psi \in \mathscr{H}_{n+2} \tag{X.52}$$

Since N is bounded from $\mathscr{H}_{n+2}$ to $\mathscr{H}_n$ and from $\mathscr{H}_{-n}$ to $\mathscr{H}_{-n-2}$, $[N, A]$ is a bounded operator from $\mathscr{H}_{n+2}$ to $\mathscr{H}_{-n-2}$. If for each $\psi \in \mathscr{H}_{n+2}$, we have that $[N, A]\psi \in \mathscr{H}_{-n}$ and

$$\|[N, A]\psi\|_{-n} \leq c\|\psi\|_n \tag{X.53}$$

then $[N, A]$ extends by the B.L.T. theorem to a bounded operator from $\mathscr{H}_n$ to $\mathscr{H}_{-n}$. In this case, we denote the extension by $[N, A]$ also.

Finally, given a quadratic form $a(\cdot, \cdot)$ on $D(N^{n/2})$, or what amounts to the same thing, an $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_{-n})$, we define an associated operator $\hat{A}$ on $\mathscr{H}$ by

$$D(\hat{A}) = \{\psi \in \mathscr{H} \cap \mathscr{H}_n \,|\, A\psi \in \mathscr{H}\}$$
$$\hat{A}\psi = A\psi, \qquad \psi \in D(\hat{A})$$

In general, $D(\hat{A})$ need not be dense. In fact, in Problem 34, the domain of $\hat{A}$ consists of just the zero vector.

We can now state the main theorem of this section. Later on (Theorem X.37) we will prove a related theorem with "operator" hypotheses rather than "form" hypotheses.

Theorem X.36 (the commutator theorem) Let N be a self-adjoint operator with $N \geq I$. Suppose that A is a symmetric operator in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ where $\mathscr{H}_n$ is the scale associated with N. Suppose that, in addition, $[N, A]$ is in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$. Then:

(a) The associated operator $\hat{A}$ is densely defined.
(b) $D(N) \subset D(\hat{A})$ and for all $\psi \in D(N)$,

$$\|\hat{A}\psi\| \leq c\|N\psi\| \tag{X.54}$$

(c) $\hat{A}$ is essentially self-adjoint on any core for N.

For clarity, we restate Theorem X.36 without mention of the scale $\mathscr{H}_n$:

Theorem X.36' Let N be a self-adjoint operator with $N \geq I$. Suppose that $a(\cdot, \cdot)$ is a quadratic form with $Q(a) = Q(N)$ so that:

(i) $|a(\psi, \varphi)| \leq c_1\|N^{1/2}\varphi\| \, \|N^{1/2}\psi\|$ for all $\varphi, \psi \in D(N^{1/2})$;
(ii) $|a(N\psi, \varphi) - a(\psi, N\varphi)| \leq c_2\|N^{1/2}\varphi\| \, \|N^{1/2}\psi\|$ for all $\varphi, \psi \in D(N^{3/2})$.

Then

(a, b') For any $\psi \in D(N)$ and all $\varphi \in D(N^{1/2})$,

$$|a(\varphi, \psi)| \leq c\|\varphi\| \, \|N\psi\|$$

so $\psi \in D(\hat{A})$ and $a(\varphi, \psi) = (\varphi, \hat{A}\psi)$ for all $\varphi \in D(N^{1/2})$ and $\hat{A}\psi$ satisfies (X.54).

(c) $\hat{A}$ is essentially self-adjoint on any core for N.

We begin the proof with two general lemmas about scales of spaces. We denote the norm in $\mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$ by $\|\cdot\|_{n,m}$.

Lemma 1 If $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$ and $[N, A] \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$, then

$$A \in \mathscr{L}(\mathscr{H}_{n+2}, \mathscr{H}_{m+2})$$

Proof Let $\psi \in \mathscr{H}_{n+2}$. A priori $NA\psi \in \mathscr{H}_{m-2}$, but $AN\psi \in \mathscr{H}_m$ since $A \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$, and $NA\psi - AN\psi \in \mathscr{H}_m$ since $[N, A] \in \mathscr{L}(\mathscr{H}_n, \mathscr{H}_m)$. Thus $NA\psi \in \mathscr{H}_m$ and

$$\begin{aligned}\|A\psi\|_{m+2} &= \|NA\psi\|_m \\ &\leq \|[N, A]\psi\|_m + \|AN\psi\|_m \\ &\leq \|[N, A]\|_{n,m}\|\psi\|_n + \|A\|_{n,m}\|N\psi\|_n \\ &\leq (\|[N, A]\|_{n,m} + \|A\|_{n,m})\|\psi\|_{n+2}\end{aligned}$$

so $A \in \mathscr{L}(\mathscr{H}_{n+2}, \mathscr{H}_{m+2})$ and

$$\|A\|_{n+2,m+2} \leq \|[N, A]\|_{n,m} + \|A\|_{n,m} \quad \blacksquare$$

Lemma 2 If $A \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ and $[N, A] \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$, then $A \in \mathscr{L}(\mathscr{H}_{+2}, \mathscr{H})$, i.e., $D(\hat{A}) \supset D(N)$ and (X.54) holds.

Proof By Lemma 1, $A \in \mathscr{L}(\mathscr{H}_{+3}, \mathscr{H}_{+1})$. Interpolating between $\mathscr{L}(\mathscr{H}_{+3}, \mathscr{H}_{+1})$ and $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ (see the Appendix to Section IX.4), we conclude that $A \in \mathscr{L}(\mathscr{H}_{+2}, \mathscr{H})$. $\blacksquare$

Proof of Theorem X.36 By Lemma 2, (a) and (b) hold. Suppose we prove that $\hat{A}$ is essentially self-adjoint on $D(N)$. Let C be a core for N. By (X.54), $\overline{\hat{A} \restriction C} \supset \hat{A} \restriction D(N)$ so $\hat{A}$ is essentially self-adjoint on C and (c) follows. Thus, we need only show that $\hat{A} \restriction D(N)$ is essentially self-adjoint. Let us denote $\hat{A} \restriction D(N)$ by B and suppose $\psi \in D(B^*)$. Then $\varphi \equiv N^{-1}\psi \in D(N) \subset D(B)$. We compute

$$\begin{aligned}|\mathrm{Im}(\varphi, B^*\psi)| &= \frac{1}{2}\,|i(\varphi, B^*\psi) - i(B^*\psi, \varphi)| \\ &= \frac{1}{2}\,|i(A\varphi, N\varphi) - i(N\varphi, A\varphi)| \\ &\leq \frac{1}{2}\,\|[N, A]\|_{+1,-1}\,\|\varphi\|_{+1}^2 \\ &\leq \frac{c}{2}\,\|\varphi\|_{+1}^2 = \frac{c}{2}\,(\varphi, \psi)\end{aligned}$$

where $c \geq \|[N, A]\|_{+1,-1}$. Thus, since (φ, ψ) is real and nonnegative,

$$\mathrm{Im}(\varphi, (\pm B^* + ic)\psi) \geq \frac{c}{2}\,(\varphi, \psi)$$

Therefore, if $(B^* \mp ic)\psi = 0$, then $(\varphi, \psi) = (\psi, N^{-1}\psi) \leq 0$. Since N^{-1} is positive with zero kernel, $\psi = 0$. We have thus proven that $\mathrm{Ker}(B^* \pm ic) = 0$, so B is essentially self-adjoint by the fundamental criterion. $\blacksquare$

An important application of Theorem X.36 appears at the end of this section. We begin here with several examples showing that certain of the hypotheses cannot be weakened.

Example 1 Let $N = p^2 + q^2$ on $L^2(\mathbb{R}, dx)$ where $p = i^{-1}\,d/dx$ and let $A = p^2 + q^2 - q^4$. By application of the methods of the Appendix to Section X.1, A is not essentially self-adjoint on $C_0^\infty(\mathbb{R})$ which is a core for N. But A and $[N, A]$ lie in $\mathscr{L}(\mathscr{H}_{+2}, \mathscr{H}_{-2})$. Thus the 1 in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ is crucial for Theorem X.36. In fact, if we take $N = (p^2 + q^2)^k$ we see that $A \in \mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ if $k \geq 2$ while $[N, A] \in \mathscr{L}(\mathscr{H}_\alpha, \mathscr{H}_{-\alpha})$ with $\alpha = 1 + k^{-1}$ (using the natural object for $\mathscr{H}_\alpha$ when α is nonintegral). Thus the ± 1 in the condition on $[N, A]$ cannot be changed even a little.

Example 2 Let $H = p^2 + q^2 + q^4$ and define $q(t) = e^{iHt}qe^{-iHt}$. Since q is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$ and $q^2 \leq cH^2$, $D(q) \supset D(H) \supset \mathscr{S}(\mathbb{R})$ and q is essentially self-adjoint on $D(H)$. Since $e^{iHt}\colon D(H) \to D(H)$, each $q(t)$ is essentially self-adjoint on $D(H)$ also. But what about $q(t_1) + q(t_2)$? This is not so easy by the methods preceding Theorem X.36. But $\pm q \leq H + 1$ so q and $q(t_1) + q(t_2)$ are in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ if $N = H$. Furthermore, $\pm i[H, q] = \pm 2p \leq 2H + 2$ so $[H, q(t_1) + q(t_2)]$ lies in $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ also. Thus, by Theorem X.36, $q(t_1) + q(t_2)$ is essentially self-adjoint on any core for H.

Example 3 Let $h(\varphi, \psi) = (\varphi, (p^2 + q^2 + \delta(q))\psi)$ on $\mathscr{S}(\mathbb{R}) \times \mathscr{S}(\mathbb{R})$. Since $\delta(q)$ is p^2-form small, the KLMN theorem guarantees a self-adjoint operator H corresponding to the form h. Let $p(t) = e^{iHt}pe^{-iHt}$. Since $[p, H]$ is badly behaved, we cannot control $p(t_1) + p(t_2)$ by the method of Example 2. However, for each real-valued $f \in C_0^\infty(\mathbb{R})$, define

$$a_f(\varphi, \psi) = \int f(t)(\varphi, p(t)\psi)\,dt, \qquad \varphi, \psi \in Q(H)$$

Then a_f is symmetric and

$$\begin{aligned}|a_f(\varphi, \varphi)| &\leq \int |f(t)|\,|(e^{-iHt}\varphi, pe^{-iHt}\varphi)|\,dt \\ &\leq \int |f(t)|\,|(e^{-iHt}\varphi, cHe^{-iHt}\varphi)|\,dt \\ &\leq ch(\varphi, \varphi)\int |f(t)|\,dt \\ &= c\|H^{1/2}\varphi\|^2\|f\|_1\end{aligned}$$

for all $\varphi \in Q(H)$. Further, for $\varphi \in D(H^2)$

$$a_f(H\varphi, \varphi) - a_f(\varphi, H\varphi) = \int f(t)\{(H\varphi, p(t)\varphi) - (\varphi, p(t)H\varphi)\}\, dt$$

$$= \int f(t) \frac{d}{dt} (\varphi, p(t)\varphi)\, dt$$

$$= -\int f'(t)(\varphi, p(t)\varphi)\, dt$$

Thus,

$$|a_f(H\varphi, \varphi) - a_f(\varphi, H\varphi)| \leq ch(\varphi, \varphi)\|f'\|_1$$
$$\leq c\|H^{1/2}\varphi\|^2\|f'\|_1$$

So, by Theorem X.36', there is a self-adjoint operator A_f associated to the quadratic form a_f and A_f is self-adjoint on any core for H. *Formally*, A_f is just $\int_{-\infty}^{\infty} f(t)p(t)\, dt$. Of course, the particular operator we have considered is not very important. What we have illustrated is that if we only know that $\pm B \leq cH$, then we can prove essential self-adjointness for

$$B_f = \int f(t)e^{iHt}Be^{-iHt}\, dt$$

for real-valued $f \in C_0^\infty(\mathbb{R})$. Such a situation arises in quantum field theory (see the references in the Notes).

Example 4 There is a connection between Theorem X.36 and a technique in the theory of ordinary differential equations. We will illustrate the technique in a case which is also easy to handle by other means. Suppose that we want to solve

$$\ddot{q}(t) = F(q(t)) \tag{X.55}$$

for a real-valued function $q(t)$ where F is some Lipschitz function obeying

$$|F(x)| \leq |x| \tag{X.56}$$

It is easy to prove local solvability of (X.55) given initial conditions (see Section V.6). To prove global solvability, we let $p = \dot{q}$ so that (X.55) becomes

$$\dot{q}(t) = p(t) \tag{X.57a}$$
$$\dot{p}(t) = F(q(t)) \tag{X.57b}$$

Let $N(p, q) = p^2 + q^2$ and let $N(t) = N(p(t), q(t))$. Suppose that we can show that for any solution on $[0, t_0)$, $N(t)$ stays bounded as $t \to t_0$. Then by a maximum interval argument similar to that used in the proof of Proposition 1 in the Appendix to X.1, we can extend the solution to $t_0 + \varepsilon$. In this way one proves that global solutions exist. To prove that $N(t)$ is bounded, we show that

$$\dot{N}(t) \leq 2N(t) \tag{X.58}$$

For

$$\dot{N}(t) = 2pF(q) + 2pq$$
$$\leq 4|pq| \leq 2N(t)$$

by (X.57) and (X.56). By integrating (X.58) we see that

$$N(t) \leq N(0)e^{2t}$$

Let us consider a formal proof of a part of Theorem X.36 based on these classical ideas. Suppose that A, N obey the hypotheses of the theorem and let $\tilde{A}$ be a self-adjoint extension, if such exists. Let $\psi \in Q(N)$ and let

$$N(t) = (\psi, e^{i\tilde{A}t}Ne^{-i\tilde{A}t}\psi)$$

Then *formally*

$$\dot{N}(t) = (e^{-i\tilde{A}t}\psi, i[A, N]e^{-i\tilde{A}t}\psi)$$
$$\leq cN(t)$$

by the bound on $i[A, N]$. This suggests that $e^{-i\tilde{A}t}$ leaves $Q(N)$ invariant which is the beginning of the self-adjointness proof of Theorem VIII.10. These formal ideas can be turned into a proof of a slightly weakened form of Theorem X.36 (see the reference in the Notes).

For our discussion of the Stark effect we need an alternative version of Theorem X.36. As it stands we need information about $D(N^{3/2})$ or $D(N^k)$ for $k \geq \frac{3}{2}$. If N is not a simple operator, it may even be very difficult to determine a core for $D(N^k)$ if $k > 1$. In such a situation the following theorem with "operator" hypotheses is useful.

Theorem X.37 Let N be a self-adjoint operator with $N \geq 1$. Let A be a symmetric *operator* with domain D which is a core for N. Suppose that:

(i) For some c and all $\varphi \in D$,

$$\|A\varphi\| \leq c\|N\varphi\| \tag{X.59}$$

(ii) For some d and all $\varphi \in D$,

$$|(A\varphi, N\varphi) - (N\varphi, A\varphi)| \leq d\|N^{1/2}\varphi\|^2 \tag{X.60}$$

Then A is essentially self-adjoint on D and its closure is essentially self-adjoint on any other core for N.

Proof By (i), the closure of A has a domain containing $D(N)$ and (ii) extends to all $\varphi \in D(N)$. By mimicking the proof of Theorem X.36 one shows that $\mathrm{Ker}(A^* \pm id) = \{0\}$ and thus A is essentially self-adjoint. ∎

We remark on one vaguely annoying feature of Theorem X.37. Namely, we need to suppose that A is an N-bounded operator and not merely an N-bounded form as in Theorem X.36. At first sight this is surprising since Lemma 2 above seems to imply that condition (ii) of Theorem X.37 and the weaker:

(i′) For some c and all $\varphi \in D$,

$$|(\varphi, A\varphi)| \leq c(\varphi, N\varphi)$$

should imply (i). The fallacy in this is that (ii) is slightly different from condition (ii) of Theorem X.36′. To have the latter we would need (X.60) for a set of φ which includes a core for $N^{3/2}$. A priori, D might be disjoint from $D(N^{3/2})$. To tantalize us, (i) implies that (ii) extends to all φ in $D(N)$ and so to $D(N^{3/2})$, but (i′) does not; so it seems impossible to use (i′) and (ii). In any event, we will need a separate argument to prove (X.59) in the following application:

Theorem X.38 (the Faris–Lavine theorem) Let V and W be real-valued measurable functions on $\mathbb{R}^n$ with

$$V(x) \geq -cx^2 - d$$

$V \in L^2_{\mathrm{loc}}(\mathbb{R}^n)$ and suppose that:

(i) There exists a dense set $D \subset D(-\Delta) \cap D(V) \cap D(W)$ which is left invariant by x_j and $i^{-1}\,\partial/\partial x_j$ so that $-\Delta + V + W + 2cx^2$ is essentially self-adjoint on D.
(ii) For some $a < 1$, $-a\Delta + W$ is bounded from below on D.

Then $-\Delta + V + W$ is essentially self-adjoint on D.

Proof By (ii) and the hypotheses on V, we can choose b so that

$$N = -\Delta + V + W + 2cx^2 + b \geq 1$$

Let $A = -\Delta + V + W$. We will verify (X.59) and (X.60) on D. As quadratic forms on D:

$$N^2 = (A + b + 2cx^2)^2 = (A + b)^2 + 4c^2x^4 + 2c(Ax^2 + x^2A) + 4bcx^2$$

$$= (A + b)^2 + 4c^2x^4 + 4c\sum_{j=1}^{n} x_j(A + b)x_j + 2c\sum_j [x_j, [x_j, A]]$$

$$= (A + b)^2 + 4c\sum_{j=1}^{n} x_j(A + b + cx^2)x_j - 4cn$$

By changing b if necessary, we can be sure that $A + b + cx^2 \geq 0$ so that

$$\|(A + b)\psi\|^2 \leq \|N\psi\|^2 + 4cn\|\psi\|^2$$

proving (X.59).

Similarly, in the sense of (X.60):

$$\pm i[A, N] = \pm i[A - N, N] = \pm i[-2cx^2, \Delta]$$
$$= \mp i4c(\mathbf{x}\cdot\nabla + \nabla\cdot\mathbf{x}) \leq 4c(-\Delta + x^2)$$
$$\leq dN$$

where we have used

$$-\Delta + x^2 \mp i(\mathbf{x}\cdot\nabla + \nabla\cdot\mathbf{x}) = (i\nabla \mp \mathbf{x})^2 \geq 0$$

and the fact that

$$N = (-a\Delta + W) + (V + cx^2) + (1 - a)(-\Delta) + cx^2$$
$$\geq e(-\Delta + x^2) - f$$

Thus by Theorem X.37, A is essentially self-adjoint on D. ∎

Corollary Let real-valued measurable functions V_1 and V_2 be given which satisfy:

(i) $V_2 \in L^p(\mathbb{R}^n)$ with $p \geq 2$ if $n \leq 3$, $p > 2$ if $n = 4$, and $p \geq n/2$ if $n \geq 5$.
(ii) $V_1 \geq -cx^2 - d$ for some c and d; $V_1 \in (L^2)_{\mathrm{loc}}$.

Then $-\Delta + V_1 + V_2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Proof Let $V = -cx^2 - d$ and $W = V_1 + V_2 + cx^2 + d$. Then by Theorem X.29, $-\Delta + W + V + 2cx^2$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ since V_2 is $-\Delta$-bounded and $V_1 + 2cx^2 + d$ is positive. Further, $-a\Delta + W$ is bounded below for any $a > 0$. Thus, by Theorem X.38, $-\Delta + V + W$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. ∎

Similarly, combining Theorem X.30, Theorem X.38, and the uncertainty principle lemma we have:

Corollary If $V(\mathbf{r}) \geq \frac{1}{4}n(4-n)r^{-2} - cr^2 - d$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n\backslash\{0\})$.

Example 5 (the Stark effect) The Hamiltonian of an atom in a constant electric field $\mathbf{E}_0$ is

$$H = -\sum_{n=1}^{N}(2m)^{-1}\Delta_n - (2M)^{-1}\Delta_0 - \sum_{n=1}^{N}\frac{Ne^2}{|\mathbf{x}_n - \mathbf{x}_0|} + \frac{1}{2}\sum_{n\neq m}\frac{e^2}{|\mathbf{x}_n - \mathbf{x}_m|} + e\mathbf{E}_0 \cdot \left(\mathbf{x}_0 - \sum_{n=1}^{N}\mathbf{x}_n\right)$$

By the first corollary, H is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3N+3})$.

By the above method one can also treat simultaneous electric and magnetic fields (see Problem 38).

X.6 Analytic vectors

Stone's theorem says that there is a one-to-one correspondence between self-adjoint operators and continuous one-parameter unitary groups. This suggests that if a symmetric operator A "determines" a unique group, then A should be essentially self-adjoint. In fact, Theorem VIII.10 says that if $U(t)$ is a continuous one-parameter unitary group, $U(t)$: $D(A) \to D(A)$ and $U'(t)\varphi = iAU(t)\varphi$ for $\varphi \in D(A)$, then A is essentially self-adjoint and generates $U(t)$. We are looking for conditions on a symmetric operator that guarantee that such a group can be constructed. The most natural way to construct $U(t)$ is to try to make sense of the power series $\sum_{n=0}^{\infty}(itA)^n/n!$ on a dense set of vectors. Notice that this can certainly be done if A is self-adjoint. For let E_Ω be the family of spectral projections for A. Then on each of the spaces $E_{[-M,M]}$, A is a bounded operator and $\sum_{n=0}^{\infty}(itA)^n/n!$ converges to e^{itA} in norm. In particular, for any $\varphi \in \bigcup_{M\geq 0} E_{[-M,M]}$,

$$\sum_{n=0}^{N}\frac{(itA)^n}{n!}\varphi \to e^{itA}\varphi$$

Since $\bigcup_{M\geq 0} E_{[-M,M]}$ is dense in $\mathscr{H}$, we see that the group generated by a self-adjoint operator A is completely determined by the well-defined action of the series $\sum_{n=0}^{\infty}(itA)^n/n!$ on a dense set. We will prove the converse: namely, if A is symmetric and has a dense set of vectors to which $\sum_{n=0}^{\infty}(itA)^n/n!$ can be applied, then A is essentially self-adjoint. We need several definitions.

Definition Let A be an operator on a Hilbert space $\mathscr{H}$. The set $C^\infty(A) \equiv \bigcap_{n=1}^{\infty} D(A^n)$ is called the **C^∞-vectors for A**. A vector $\varphi \in C^\infty(A)$ is called an **analytic vector for A** if

$$\sum_{n=0}^{\infty}\frac{\|A^n\varphi\|}{n!}t^n < \infty$$

for some $t > 0$.

If A is self-adjoint, then $C^\infty(A)$ will be dense in $D(A)$. However, in general, a symmetric operator may have no C^∞ vectors at all even if A is essentially self-adjoint. We caution the reader to remember that analytic vectors and vectors of uniqueness (defined below) must be C^∞ vectors for A. A vector $\psi \in D(A)$ can be an analytic vector for an extension of A but fail to be an analytic vector for A because it is not in $C^\infty(A)$.

Definition Suppose that A is symmetric. For each $\varphi \in C^\infty(A)$, define

$$D_\varphi = \left\{ \sum_{n=0}^{N}\alpha_n A^n\varphi \,\middle|\, N = 1, 2, \ldots, \langle\alpha_1, \ldots, \alpha_N\rangle \text{ arbitrary} \right\}$$

Let $\mathscr{H}_\varphi = \overline{D}_\varphi$ and define $A_\varphi : D_\varphi \to D_\varphi$ by $A_\varphi(\sum_{n=0}^{N}\alpha_n A^n\varphi) = \sum_{n=0}^{N}\alpha_n A^{n+1}\varphi$. φ is called a **vector of uniqueness** if and only if A_φ is essentially self-adjoint on D_φ (as an operator on $\mathscr{H}_\varphi$).

Finally, a subset S of $\mathscr{H}$ is called **total** if the set of finite linear combinations of elements of S is dense in $\mathscr{H}$.

Lemma (Nussbaum) Let A be a symmetric operator and suppose that $D(A)$ contains a total set of vectors of uniqueness. Then A is essentially self-adjoint.

Proof We will show that $\mathrm{Ran}(A \pm i)$ are dense in $\mathscr{H}$. By the fundamental criterion this will show that A is essentially self-adjoint. Suppose $\psi \in \mathscr{H}$ and $\varepsilon > 0$ are given and let S denote the set of vectors of uniqueness. Since S is total we can find $\langle\alpha_1, \ldots, \alpha_N\rangle$ and $\langle\psi_1, \ldots, \psi_N\rangle$ with $\psi_n \in S$ so

that $\|\psi - \sum_{n=1}^{N} \alpha_n \psi_n\| \leq \varepsilon/2$. Since ψ_n is a vector of uniqueness, there is a $\varphi_n \in D_{\psi_n}$ so that

$$\|\psi_n - (A + i)\varphi_n\| \leq \frac{\varepsilon}{2}\left(\sum_{n=1}^{N} |\alpha_n|\right)^{-1}$$

Setting $\varphi = \sum_{n=1}^{N} \alpha_n \varphi_n$, we have $\varphi \in D(A)$ and $\|\psi - (A + i)\varphi\| \leq \varepsilon$. Thus $\mathrm{Ran}(A + i)$ is dense. The proof for $(A - i)$ is the same. ∎

Theorem X.39 (Nelson's analytic vector theorem) Let A be a symmetric operator on a Hilbert space $\mathscr{H}$. If $D(A)$ contains a total set of analytic vectors, then A is essentially self-adjoint.

Proof By Nussbaum's lemma, it is enough to show that each analytic vector ψ is a vector of uniqueness. First notice that by Theorem X.3, A_ψ always has self-adjoint extensions, since the operator

$$C: \sum_{n=0}^{N} \alpha_n A^n \psi \to \sum_{n=0}^{N} \bar{\alpha}_n A^n \psi$$

extends to a conjugation on $\mathscr{H}_\psi$ which commutes with A_ψ. Suppose that B is a self-adjoint extension of A_ψ on $\mathscr{H}_\psi$ and let μ be the spectral measure for B associated to ψ. Since ψ is an analytic vector for A, $\sum_{n=0}^{\infty} (\|A^n\psi\|/n!)t^n < \infty$ for some $t > 0$. Let $0 < s < t$. Then

$$\sum_{n=0}^{\infty} \frac{s^n}{n!} \int_{-\infty}^{\infty} |x|^n \, d\mu \leq \sum_{n=0}^{\infty} \frac{s^n}{n!} \left(\int_{-\infty}^{\infty} x^{2n} \, d\mu\right)^{1/2} \left(\int_{-\infty}^{\infty} d\mu\right)^{1/2}$$

$$= \|\psi\| \sum_{n=0}^{\infty} \frac{s^n}{n!} \|A^n\psi\| < \infty$$

Thus, by Fubini's theorem,

$$\int_{-\infty}^{\infty} \sum_{n=0}^{\infty} \frac{s^n}{n!} |x|^n \, d\mu = \int_{-\infty}^{\infty} e^{s|x|} \, d\mu < \infty$$

As a result, the function $(\psi, e^{itB}\psi) = \int_{-\infty}^{\infty} e^{itx} \, d\mu$ has an analytic continuation $\int_{-\infty}^{\infty} e^{izx} \, d\mu$ to the region $|\mathrm{Im}\, z| < t$. Since

$$\left[\left(\frac{d}{dz}\right)^k \int_{-\infty}^{\infty} e^{izx} \, d\mu\right]_{z=0} = \int_{-\infty}^{\infty} (ix)^k \, d\mu = (\psi, (iA)^k\psi)$$

we have

$$(\psi, e^{isB}\psi) = \sum_{n=0}^{\infty} \frac{(is)^n}{n!} (\psi, A^n\psi)$$

for $|s| < t$. Thus, for $|s| < t$ (and therefore for all s), the function $(\psi, e^{isB}\psi)$ is completely determined by the numbers $(\psi, A^n\psi)$, $n = 0, 1, 2, \ldots$. A

similar proof shows that $(\psi_1, e^{isB}\psi_2)$ is determined by the numbers $(\psi_1, A^n\psi_2)$, $n = 0, 1, 2, \ldots$, for any $\psi_1, \psi_2 \in D_\psi$. Since D_ψ is dense in $\mathscr{H}_\psi$ and e^{isB} is unitary, e^{isB} is completely determined by the numbers $(\psi_1, A^n\psi_2)$ for $\psi_1, \psi_2 \in D_\psi$ and $n = 0, 1, 2, \ldots$. Thus, all self-adjoint extensions of A_ψ generate the same unitary group, so by Stone's theorem A_ψ has at most one self-adjoint extension. As we have already remarked, A_ψ has at least one self-adjoint extension. Thus A_ψ is essentially self-adjoint and ψ is a vector of uniqueness. ∎

Corollary 1 A closed symmetric operator A is self-adjoint if and only if $D(A)$ contains a dense set of analytic vectors.

The statement of Corollary 1 is not true if "self-adjoint" is replaced by "essentially self-adjoint." A self-adjoint operator A may be essentially self-adjoint on a domain $D \subset D(A)$ and D may not even contain any C^∞ vectors. The reader is asked to construct an example in Problem 39.

Corollary 2 Suppose that A is a symmetric operator and let D be a dense linear set contained in $D(A)$. Then, if D contains a dense set of analytic vectors *and if D is invariant under A*, then A is essentially self-adjoint on D.

Proof Since D is invariant under A, each analytic vector for A in D is also an analytic vector for $A \restriction D$. Thus, by Theorem X.39 $A \restriction D$ is essentially self-adjoint. ∎

The reason that one needs the invariance condition in Corollary 2 is that for a vector $\psi \in D$ to be analytic for $A \restriction D$, it must first be C^∞ for $A \restriction D$. This requires that $A^n\psi \in D$ for all n. The following is a simple example which shows why one must be very careful of this invariance condition.

Example 1 Let $\mathscr{H} = \ell_2$ and let A be the self-adjoint operator which has the vectors $\delta_n = \langle 0, 0, \ldots, 1, 0, 0, \ldots \rangle$ as eigenfunctions with $A\delta_n = n\delta_n$. By Proposition 1 of Section VIII.3, $D(A) = \{\{a_n\} | \{na_n\} \in \ell_2\}$. Now, let $D = \{\sum_{n=1}^{N} \alpha_n \delta_n | \sum \alpha_n = 0, N \text{ arbitrary but finite}\}$. First, it is clear that each vector in D is an analytic vector for A, since $\|A^k \sum_{n=1}^{N} \alpha_n \delta_n\|^2 \leq N^{2k} \sum_{n=1}^{N} |\alpha_n|^2$. Secondly, D is dense in ℓ_2. For, suppose that $\{a_n\}$ is a sequence in ℓ_2 which is zero after the Mth place. Then the vector

$$\varphi = \Big\langle a_1, \ldots, a_M, \underbrace{\frac{-\sum_{i=1}^{M} a_i}{k}, \ldots, \frac{-\sum_{i=1}^{M} a_i}{k}}_{k \text{ places}}, 0, \ldots \Big\rangle$$

is in D and satisfies

$$\|\{a_n\} - \varphi\|_{\ell_2} \leq \left| \sum_{i=1}^{N} a_i \right| k^{-1/2}$$

Thus $\{a_n\}$ can be approximated by elements of D. Since the set of such $\{a_n\}$ are dense, so is D.

Thus, D is a dense set of analytic vectors for A, But, $A \restriction D$ is *not* essentially self-adjoint. For, let $\psi = \{1/n\}_{n=1}^{\infty}$. Then, for all $\varphi \in D$, $(A\varphi, \psi) = 0$. So, $\psi \in D((A \restriction D)^*)$ and $(A \restriction D)^*\psi = 0$. This shows that $D((N \restriction D)^*)$ *strictly* contains $D(A)$, so A is not essentially self-adjoint on D. Notice, that A does not take D into itself.

The following examples illustrate in a simple way how analytic vectors can be used. Some applications of analytic vectors in quantum field theory are described in the next section.

Example 2 Let A and $A^\dagger$ be the maps of $\mathscr{S}(R)$ into itself given by

$$A = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right), \qquad A^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right)$$

and define $N = A^\dagger A$. Let $\phi_0 = \pi^{-1/4}e^{-x^2/2}$ and $\phi_n = (n!)^{-1/2}(A^\dagger)^n\phi_0$. The ϕ_n are just the Hermite functions which form an orthonormal basis for $L^2(\mathbb{R})$ (see Problems 6 and 7 of Chapter IX). The operator N satisfies $N\phi_n = n\phi_n$ and A and $A^\dagger$ satisfy the commutation relation (on $\mathscr{S}(\mathbb{R})$):

$$AA^\dagger - A^\dagger A = I$$

It follows easily that $A^\dagger\phi_n = \sqrt{n+1}\,\phi_{n+1}$ and $A\phi_n = \sqrt{n}\,\phi_{n-1}$ if $n \geq 1$, and $A\phi_0 = 0$. Therefore

$$\|\underbrace{A^\# A^\# \cdots A^\#}_{k \text{ times}}\phi_n\| \leq (n+1)^{1/2} \cdots (n+k)^{1/2} \leq [(n+k)!]^{1/2} \quad \text{(X.61)}$$

where each $A^\#$ can represent either A or $A^\dagger$. Since $x^k = 2^{-k/2}(A + A^\dagger)^k$, (X.61) implies

$$\|x^k\phi_n\| \leq 2^{k/2}[(n+k)!]^{1/2}$$

and therefore

$$\sum_{k=0}^{\infty} \frac{\|x^k\phi_n\|}{k!} t^k \leq \sum_{k=0}^{\infty} \frac{2^{k/2}[(n+k)!]^{1/2}}{k!} t^k < \infty$$

for all t so each ϕ_n is an analytic vector for x. Since the set of finite linear combinations of the Hermite functions is a dense set invariant under x, we conclude that x is essentially self-adjoint on any linear subspace of $L^2(\mathbb{R})$ contained in $\{\varphi \mid \|x\varphi\|_2 < \infty\}$ which contains the Hermite functions. A similar statement holds for $i\,d/dx$.

Example 3 Let A_n be a self-adjoint operator on $\mathscr{H}_n$, $n = 1, 2, \ldots, N$, and suppose that $P(x_1, \ldots, x_N)$ is a polynomial with real coefficients of degree n_k in x_k. Let D_k^e be a domain of essential self-adjointness for A_k. Under these hypotheses, we proved in Theorem VIII.33 that the operator $P(A_1, \ldots, A_N)$ on $\mathscr{H}_1 \otimes \cdots \otimes \mathscr{H}_N$ is essentially self-adjoint on

$$D^e = \bigotimes_{n=1}^{N} D_n^e$$

The proof given in Theorem VIII.33 depended on the spectral theorem. Here we will give another proof which uses analytic vectors. $P(A_1, \ldots, A_N)$ is clearly symmetric on $D^e = \otimes_{n=1}^{N} D_k^e$. Further, since $\overline{A_n \restriction D_n^e} = A_n$, the closure of $P(A_1, \ldots, A_N)$ on D^e is the same as the closure of $P(A_1, \ldots, A_N)$ on $D = \otimes_{n=1}^{N} D(A_k)$. Therefore, it suffices to prove that $P(A_1, \ldots, A_N)$ is essentially self-adjoint on D. Let E_Ω^n be the projection-valued measure of A_n and suppose that M_n, $n = 1, \ldots, N$, are nonnegative numbers. Let $\varphi_n \in E^n_{[-M_n, M_n]}\mathscr{H}_n$; then $\|A_n\varphi_n\| \leq M_n\|\varphi_n\|$ and if $\varphi = \varphi_1 \otimes \cdots \otimes \varphi_N$ a short calculation shows that

$$\|[P(A_1, \ldots, A_N)]^k\varphi\| \leq (\tilde{P}(M_1, \ldots, M_N))^k\|\varphi\|$$

where the $\tilde{P}$ is the same polynomial as P except that each coefficient has been replaced by its absolute value. This implies that

$$\sum_{k=0}^{\infty} \frac{\|P(A_1, \ldots, A_N)^k\varphi\|}{k!} t^k < \infty$$

for all t so φ is an analytic vector for $P(A_1, \ldots, A_N)$. The set of finite linear combinations of such vectors is invariant under $P(A_1, \ldots, A_N)$ and is a dense subset of D. Thus, by Nelson's theorem, $P(A_1, \ldots, A_N)$ is essentially self-adjoint on D and therefore also on D^e (as remarked above).

Example 4 (Hamburger moment problem—uniqueness) In Example 3 of Section X.1 we proved a theorem giving necessary and sufficient conditions on a sequence of real numbers so that $a_n = \int_{\mathbb{R}} x^k\,d\rho(x)$ for some positive measure ρ. We will use the notation of that example. Suppose that there exist constants C and D so that $|a_n| \leq CD^n n!$ for all n. Since $\hat{A}$: $P/Q \to P/Q$,

each vector in P/Q is a C^∞ vector for $\hat{A}$. The bounds on $\{a_n\}$ thus immediately imply that P/Q is a dense set of analytic vectors for $\hat{A}$. By Theorem X.39, $\hat{A}$ is essentially self-adjoint on P/Q and thus $\hat{A} = \tilde{A}$.

Therefore $\tilde{A}$ and thus the measure ρ are uniquely determined by the sequence $\{a_n\}$. Thus in the case where $|a_n| \leq CD^n n!$, we have proven that the Hamburger moment problem has a unique solution.

Various extensions of Nelson's theorem are discussed in the Notes. The reader can prove (Problem 42) the following extension in the semibounded case by using methods similar to those used above.

Definition Let A be an operator on a Hilbert space $\mathscr{H}$. A vector $\varphi \in C^\infty(A)$ is called a **semianalytic** vector for A if

$$\sum_{n=0}^{\infty} \frac{\|A^n \varphi\|}{(2n)!} t^n < \infty$$

for some $t > 0$.

Theorem X.40 Let A be a *semibounded* symmetric operator. If $D(A)$ contains a total set of semianalytic vectors, then A is essentially self-adjoint.

Theorem X.40 has two corollaries analogous to the corollaries of Theorem X.39.

Example 5 (essential self-adjointness of $H = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4/4$; third proof) In terms of the notation introduced in Example 2, $H = A^\dagger A + (A^\dagger + A)^4$. Let ϕ_n be the nth Hermite function. H^k has 17^k terms each of them a product of less than or equal to $4k$ operators $A^\dagger$ or A. Thus, using (X.61) we have

$$\begin{aligned} \|H^k \phi_n\| &\leq 17^k (n+1)^{1/2} \cdots (n+4k)^{1/2} \\ &\leq 17^k 2^{2k} (2k)^{2k} c_n \end{aligned}$$

Thus, the Hermite functions are a total set of semianalytic vectors for H with domain $\mathscr{S}(\mathbb{R})$. Therefore, by Theorem X.40, H is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, since H is clearly nonnegative.

Example 6 Using Theorem X.40 one can prove, similarly to Example 4, that the Stieltjes moment problem has a unique solution if $|a_n| \leq CD^n(2n)!$ for some constants C and D. See Problem 25.

X.7 Free quantum fields

First quantization is a mystery, but second quantization is a functor. — *E. Nelson*

In Section IX.8, we described the Wightman axioms for a single scalar quantum field. In this section, we continue our discussion of quantum field theory. First, we introduce the abstract free field and use it to construct explicitly a family of examples satisfying the Wightman axioms: for each $m > 0$, we construct the free scalar field of mass m. These theories are inequivalent in the sense that there does not exist a unitary map from one Hilbert space to the other which preserves all the field theory structures (vacuum, fields, etc.). A stronger sense in which these theories are inequivalent is that the time-zero fields give different representations of the canonical commutation relations (see the Appendix to this section). In addition to proving that the axioms are satisfied, we will show that the fields are self-adjoint. The main tool in this self-adjointness proof is the analytic vector theorem.

As the name suggests, the free scalar field theories describe noninteracting particles. Nevertheless, they are important since they show that the Wightman axioms are consistent and because the most natural way to construct "interacting" theories is to make perturbations of the free theories. In the second part of this section we begin our discussion of the simplest interacting theory, the φ^4 self-interaction in two-dimensional space–time. We introduce the spatially cut-off Hamiltonian $H(g)$ and show that it is a symmetric operator. Finally, we introduce Q-space, a reformulation of the Fock space structures, which we use in Section X.9 where we prove that $H(g)$ is self-adjoint. We will *not* conclude the construction of these interacting field theories to the point of removing the spatial cut-off and proving the Wightman axioms. This has been done for a class of models; see the references in the Notes.

Let $\mathscr{H}$ be a complex Hilbert space and let $\mathscr{F}(\mathscr{H}) = \bigoplus_{n=0}^{\infty} \mathscr{H}^{(n)}$ (where $\mathscr{H}^{(n)} = \bigotimes_{k=1}^{n} \mathscr{H}$) be the Fock space over $\mathscr{H}$ defined in Section II.4. Our goal is to define the abstract free field on $\mathscr{F}_s(\mathscr{H})$, the Boson subspace of $\mathscr{F}(\mathscr{H})$; to do this we need to introduce several other families of operators and some terminology. Let $f \in \mathscr{H}$ be fixed. For vectors in $\mathscr{H}^{(n)}$ of the form $\eta = \psi_1 \otimes \cdots \otimes \psi_n$ we define a map $b^-(f)$: $\mathscr{H}^{(n)} \to \mathscr{H}^{(n-1)}$ by

$$b^-(f)\eta = (f, \psi_1)(\psi_2 \otimes \cdots \otimes \psi_n)$$

$b^-(f)$ extends by linearity to finite linear combinations of such η, the extension is well defined, and $\|b^-(f)\eta\| \leq \|f\| \, \|\eta\|$. Thus $b^-(f)$ extends to a bounded map (of norm $\|f\|$) of $\mathscr{H}^{(n)}$ into $\mathscr{H}^{(n-1)}$. Since this is true

for each n (except for $n=0$ in which case we define $b^-(f)$: $\mathscr{H}^{(0)} \to 0$), $b^-(f)$ is in a natural way a bounded operator of norm $\|f\|$ from $\mathscr{F}(\mathscr{H})$ to $\mathscr{F}(\mathscr{H})$. It is easy to check that $b^+(f) \equiv (b^-(f))^*$ takes each $\mathscr{H}^{(n)}$ into $\mathscr{H}^{(n+1)}$ with the action

$$b^+(f)(\psi_1 \otimes \cdots \otimes \psi_n) = f \otimes \psi_1 \otimes \cdots \otimes \psi_n$$

on product vectors. Notice that the map $f \mapsto b^+(f)$ is linear, but $f \mapsto b^-(f)$ is antilinear.

Let S_n be the symmetrization operators introduced in Section II.4. Then $S = \oplus_{n=0}^{\infty} S_n$ is the projection onto the symmetric Fock space $\mathscr{F}_s(\mathscr{H}) \equiv \oplus_{n=0}^{\infty} S_n \mathscr{H}^{(n)}$. We will write $S_n \mathscr{H}^{(n)} \equiv \mathscr{H}_s^{(n)}$ and call $\mathscr{H}_s^{(n)}$ the ***n*-particle subspace of** $\mathscr{F}_s(\mathscr{H})$. Notice that $b^-(f)$ takes $\mathscr{F}_s(\mathscr{H})$ into itself, but that $b^+(f)$ does not. A vector $\psi = \{\psi^{(n)}\}_{n=0}^{\infty} \in \mathscr{F}_s(\mathscr{H})$ for which $\psi^{(n)} = 0$ for all but finitely many n is called a **finite particle vector**. We will denote the set of finite particle vectors by F_0. The vector $\Omega_0 = \langle 1, 0, 0, \ldots \rangle$ plays a special role; it is called the **vacuum**.

Let A be any self-adjoint operator on $\mathscr{H}$ with domain of essential self-adjointness D. Let $D_A = \{\psi \in F_0 \,|\, \psi^{(n)} \in \otimes_{k=1}^{n} D \text{ for each } n\}$ and define $d\Gamma(A)$ on $D_A \cap \mathscr{H}_s^{(n)}$ as

$$A \otimes I \otimes \cdots \otimes I + I \otimes A \otimes \cdots \otimes I + \cdots + I \otimes \cdots \otimes I \otimes A$$

In Section VIII.10, we proved that $d\Gamma(A)$ is essentially self-adjoint on D_A; $d\Gamma(A)$ is called the **second quantization** of A. For example, let $A = I$. Then its second quantization $N = d\Gamma(I)$ is essentially self-adjoint on F_0 and for $\psi \in \mathscr{H}_s^{(n)}$, $N\psi = n\psi$. N is called the **number operator**. If U is a unitary operator on $\mathscr{H}$, we define $\Gamma(U)$ to be the unitary operator on $\mathscr{F}_s(\mathscr{H})$ which equals $\otimes_{k=1}^{n} U$ when restricted to $\mathscr{H}_s^{(n)}$ for $n > 0$, and which equals the identity on $\mathscr{H}_s^{(0)}$. If e^{itA} is a continuous unitary group on $\mathscr{H}$, then $\Gamma(e^{itA})$ is the group generated by $d\Gamma(A)$, i.e., $\Gamma(e^{itA}) = e^{itd\Gamma(A)}$.

We now define the **annihilation operator** $a^-(f)$ on $\mathscr{F}_s(\mathscr{H})$ with domain F_0 by

$$a^-(f) = \sqrt{N+1}\, b^-(f) \tag{X.62}$$

$a^-(f)$ is called an annihilation operator because it takes each $(n+1)$-particle subspace into the n-particle subspace. For each ψ and η in F_0,

$$(\sqrt{N+1}\, b^-(f)\psi, \eta) = (\psi, Sb^+(f)\sqrt{N+1}\,\eta)$$

This implies that

$$(a^-(f))^* \restriction F_0 = Sb^+(f)\sqrt{N+1} \tag{X.63}$$

The operator $(a^-(f))^*$ is called a **creation operator**. Both $a^-(f)$ and $a^-(f)^* \restriction F_0$ are closable; we denote their closures by $a^-(f)$ and $a^-(f)^*$ also.

Example 1 If $\mathscr{H} = L^2(M, d\mu)$, we have seen in Section II.4 that

$$\bigotimes_{j=1}^{n} L^2(M, d\mu) = L^2(M \times \cdots \times M, d\mu \otimes \cdots \otimes d\mu)$$

and that

$$S \bigotimes_{j=1}^{n} L^2(M, d\mu) = L_s^2(M \times \cdots \times M, d\mu \otimes \cdots \otimes d\mu)$$

where L_s^2 is the set of functions in L^2 which are invariant under permutations of the coordinates. The operators $a^-(f)$ and $a^-(f)^*$ are given by

$$(a^-(f)\psi)^{(n)}(m_1, \ldots, m_n) = \sqrt{n+1} \int_M \bar{f}(m)\psi^{(n+1)}(m, m_1, \ldots, m_n)\, d\mu(m)$$

$$(a^-(f)^*\psi)^{(n)}(m_1, \ldots, m_n) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} f(m_i)\psi^{(n-1)}(m_1, \ldots, \hat{m}_i, \ldots, m_n)$$

where $\hat{m}_i$ means that m_i is omitted. If A operates on $L^2(M, d\mu)$ by multiplication by the real-valued function $\omega(m)$, then

$$(d\Gamma(A)\psi)^{(n)}(m_1, \ldots, m_n) = \left(\sum_{i=1}^{n} \omega(m_i)\right)\psi^{(n)}(m_1, \ldots, m_n)$$

(X.63) implies that the **Segal field operator** $\Phi_S(f)$ on F_0 defined by

$$\Phi_S(f) = \frac{1}{\sqrt{2}}(a^-(f) + a^-(f)^*)$$

is symmetric. In fact, we will shortly see that $\Phi_S(f)$ is essentially self-adjoint. The mapping from $\mathscr{H}$ to the self-adjoint operators on $\mathscr{F}_s(\mathscr{H})$ given by

$$f \mapsto \Phi_S(f)$$

is called the **Segal quantization over** $\mathscr{H}$. Notice that the Segal quantization is a real (*but not complex*) linear map since $f \mapsto a^-(f)$ is antilinear and $f \mapsto (a^-(f))^*$ is linear. The following theorem gives the fundamental properties of the Segal quantization.

Theorem X.41 Let $\mathscr{H}$ be a complex Hilbert space; $\Phi_S(\cdot)$ the corresponding Segal quantization. Then:

(a) (self-adjointness) For each $f \in \mathscr{H}$, $\Phi_S(f)$ is essentially self-adjoint on F_0, the finite particle vectors.

(b) (cyclicity of the vacuum) Ω_0 is in the domain of all finite products $\Phi_S(f_1)\cdots\Phi_S(f_n)$ and the set $\{\Phi_S(f_1)\cdots\Phi_S(f_n)\Omega_0 \mid f_i \text{ and } n \text{ arbitrary}\}$ is total in $\mathscr{F}_s(\mathscr{H})$.

(c) (commutation relations) For each $\psi \in F_0$ and $f, g \in \mathscr{H}$,

$$\Phi_S(f)\Phi_S(g)\psi - \Phi_S(g)\Phi_S(f)\psi = i\,\mathrm{Im}(f,g)_{\mathscr{H}}\psi \tag{X.64}$$

Further, if $W(f)$ denotes the unitary operator $e^{i\Phi_S(f)}$, then

$$W(f+g) = e^{-i\,\mathrm{Im}(f,g)/2}W(f)W(g) \tag{X.65}$$

(d) (continuity) If $f_n \to f$ in $\mathscr{H}$, then

$$W(f_n)\psi \to W(f)\psi \qquad \text{for all } \psi \in \mathscr{F}_s(\mathscr{H})$$
$$\Phi_S(f_n)\psi \to \Phi_S(f)\psi \qquad \text{for all } \psi \in F_0$$

(e) For every unitary operator U on $\mathscr{H}$, $\Gamma(U)$: $D(\overline{\Phi_S(f)}) \to D(\overline{\Phi_S(Uf)})$ and for $\psi \in D(\overline{\Phi_S(Uf)})$,

$$\Gamma(U)\overline{\Phi_S(f)}\Gamma(U)^{-1}\psi = \overline{\Phi_S(Uf)}\psi$$

for all $f \in \mathscr{H}$.

Proof Let $\psi \in \mathscr{H}_s^{(n)}$. Since $\Phi_S(f)$: $F_0 \to F_0$, ψ is in $C^\infty(\Phi_S(f))$. Further, it follows from (X.62), (X.63), and the fact that $\|b^-(f)\| = \|f\|$, that

$$\|\underbrace{a^\#(f)\cdots a^\#(f)}_{k \text{ times}}\psi\| \le \sqrt{n+1}\cdots\sqrt{n+k}\,\|f\|^k\,\|\psi\|$$

where $a^\#(f)$ represents either $a^-(f)$ or $(a^-(f))^*$. Therefore,

$$\|(\Phi_S(f))^k\psi\| \le 2^{k/2}((n+k)!)^{1/2}\|f\|^k\|\psi\|$$

Since $\sum_{k=0}^\infty t^k 2^{k/2}((n+k)!)^{1/2}\|f\|^k/k! < \infty$ for all t, ψ is an analytic vector for $\Phi_S(f)$. Since F_0 is dense in $\mathscr{F}_s(\mathscr{H})$ and is left invariant by Φ_S, $\Phi_S(f)$ is essentially self-adjoint on F_0 by Nelson's analytic vector theorem (Theorem X.39).

The proof of (b) is left as Problem 43.

To prove (c) one first computes that if $\psi \in F_0$, then

$$a^-(f)a^-(g)^*\psi - a^-(g)^*a^-(f)\psi = (f,g)\psi \tag{X.66}$$

(X.64) follows immediately. Although (X.64) and (X.65) are formally equivalent, (X.64) by itself does not imply (X.65) (for an example of how misleading such formal calculations can be, see Section VIII.5). We sketch a proof of (X.65) which uses special properties of the vectors in F_0.

Let $\psi \in \mathscr{H}_s^{(p)}$. Then

$$\|\Phi_S(f)^n\Phi_S(g)^m\psi\| \le 2^{(n+m)/2}\sqrt{p+1}\cdots\sqrt{p+n+m}\,\|f\|^n\|g\|^m\|\psi\|$$

which implies that $\sum_{n,m}(\|\Phi_S(f)^n\Phi_S(g)^m\psi\|/n!\,m!)t^nt^m$ converges for all t. Since ψ is an analytic vector for $\Phi_S(g)$, $\sum_m((i\Phi_S(g))^m/m!)\psi = e^{i\Phi_S(g)}\psi$. Further, for each n, $e^{i\Phi_S(g)}\psi$ is in the domain of $\overline{(\Phi_S(f))^n}$ since

$$\sum_{m=0}^{M}\frac{(i\Phi_S(g))^m}{m!}\psi$$

is in it and $\Phi_S(f)^n\sum_{m=0}^M((i\Phi_S(g))^m/m!)\psi$ converges as $M \to \infty$. Thus the estimate

$$\sum_{n,m}\frac{\|(\Phi_S(f))^n(\Phi_S(g))^m\|}{n!\,m!}t^nt^m < \infty$$

shows that $e^{i\Phi_S(g)}\psi$ is an analytic vector for $\Phi_S(f)$ and therefore $e^{i\Phi_S(f)}$ can be computed by the power series. Thus

$$e^{i\Phi_S(f)}e^{i\Phi_S(g)}\psi = \sum_{n,m}\frac{(i\Phi_S(f))^n(i\Phi_S(g))^m}{n!\,m!}\psi$$

Similarly,

$$e^{-it^2\,\mathrm{Im}(f,g)/2}e^{it\Phi_S(f+g)}\psi = \sum_{n,m=0}^{\infty}\frac{1}{m!}\frac{1}{n!}\left[\left(-\frac{it^2}{2}\mathrm{Im}(f,g)\right)^m(it\Phi_S(f+g))^n\right]\psi$$

converges absolutely. Direct computations using (X.64) now show that (X.65) holds by a term-by-term comparison of the convergent power series.

To prove (d) let $\psi \in \mathscr{H}_s^{(k)}$ and suppose that $f_n \xrightarrow{\mathscr{H}} f$. Then

$$\|\Phi_S(f_n)\psi - \Phi_S(f)\psi\| \le \sqrt{2}\sqrt{k+1}\,\|f_n - f\|\,\|\psi\|$$

so $\Phi_S(f_n)\psi \to \Phi_S(f)\psi$. Thus, $\Phi_S(f_n)$ converges strongly to $\Phi_S(f)$ on F_0. Since F_0 is a core for all $\Phi_S(f_n)$ and $\Phi_S(f)$, Theorems VIII.21 and VIII.25 imply that $e^{it\Phi_S(f_n)}\psi \to e^{it\Phi_S(f)}\psi$ for all $\psi \in \mathscr{F}_s(\mathscr{H})$.

To prove (e), let $\eta \in \mathscr{H}^{(n)}$ be of the form $\eta = \psi_1 \otimes \cdots \otimes \psi_n$. Then

$$\begin{aligned}\Gamma(U)b^-(f)\Gamma(U)^{-1}\eta &= \Gamma(U)b^-(f)(U^{-1}\psi_2 \otimes \cdots \otimes U^{-1}\psi_n)\\ &= \Gamma(U)(f, U^{-1}\psi_1)(U^{-1}\psi_2 \otimes \cdots \otimes U^{-1}\psi_n)\\ &= (Uf, \psi_1)(\psi_2 \otimes \cdots \otimes \psi_n)\\ &= b^-(Uf)\eta\end{aligned}$$

Since finite linear combinations of such η are dense in $\mathscr{H}^{(n)}$ and $b^-(g)$ has norm $\|g\|$, we conclude that $\Gamma(U)b^-(f)\Gamma(U)^{-1} = b^-(Uf)$. But N and S commute with $\Gamma(U)$, so this immediately implies that $\Gamma(U)a^-(f)\Gamma(U)^{-1} = a^-(Uf)$ on F_0. Taking adjoints and restricting to F_0 we also have $\Gamma(U)(a^-(f))^*\Gamma(U)^{-1} = (a^-(Uf))^*$. Thus, for $\psi \in F_0$, $\Gamma(U)\Phi_S(f)\Gamma(U)^{-1}\psi = \Phi_S(Uf)\psi$. Since the operators on both the right- and left-hand sides of this equality are essentially self-adjoint on F_0, we conclude that

$$\Gamma(U)\overline{\Phi_S(f)}\Gamma(U)^{-1} = \overline{\Phi_S(Uf)} \quad \blacksquare$$

Henceforth we use $\Phi_S(f)$ to denote the closure of $\Phi_S(f)$.

We can now use the Segal quantization to define the free Hermitian scalar field of mass m. We take $\mathscr{H} = L^2(H_m, d\Omega_m)$, where H_m, $m \geq 0$, is the mass hyperboloid in $\mathbb{R}^4$ consisting of those $p \in \mathbb{R}^4$ satisfying $p \cdot \tilde{p} - m^2 = 0$ and $p_0 > 0$, and Ω_m is the Lorentz invariant measure (defined in Section IX.8). For each $f \in \mathscr{S}(\mathbb{R}^4)$ we define Ef in $\mathscr{H}$ by $Ef = \sqrt{2\pi}\hat{f} \restriction H_m$ where (for this section only) the Fourier transform

$$\hat{f}(p) = \frac{1}{(2\pi)^2}\int e^{ip\cdot\tilde{x}} f(x)\, dx$$

is defined in terms of the Lorentz invariant inner product $p \cdot \tilde{x}$. The reason for the extra $\sqrt{2\pi}$ in our definition of E and the plus sign in the definition of Fourier transform is that if f is the distribution $f(x) = g(\mathbf{x})\delta(t)$, then $\sqrt{2\pi}\,\hat{f}$ is the ordinary three-dimensional Fourier transform of g. If $\Phi_S(\cdot)$ is the Segal quantization over $L^2(H_m, d\Omega_m)$, we define for each *real-valued* $f \in \mathscr{S}(\mathbb{R}^4)$

$$\Phi_m(f) = \Phi_S(Ef) \tag{X.67a}$$

For arbitrary $f \in \mathscr{S}(\mathbb{R}^4)$, we define

$$\Phi_m(f) = \Phi_m(\mathrm{Re}\ f) + i\Phi_m(\mathrm{Im}\ f) \tag{X.67b}$$

The mapping $f \mapsto \Phi_m(f)$ is called the **free Hermitian scalar field of mass m.**

On $L^2(H_m, d\Omega_m)$ we define the following unitary representation of the restricted Poincaré group:

$$(U_m(a, \Lambda)\psi)(p) = e^{ip\cdot\tilde{a}}\psi(\Lambda^{-1}p) \tag{X.68}$$

where we are using Λ to denote both an element of the abstract restricted Lorentz group and the corresponding element in the standard representation on $\mathbb{R}^4$. As before F_0 will denote the finite particle vectors.

Theorem X.42 The quadruple

$$\langle \mathscr{F}_s(L^2(H_m, d\Omega_m)), \Gamma(U_m(\cdot,\cdot)), \Phi_m(\cdot), F_0\rangle$$

satisfies the Wightman axioms. Further, for each $f \in \mathscr{S}(\mathbb{R}^4)$,

$$\Phi_m((\Box^2 + m^2)f) = 0$$

where $\Box^2 = \partial^2/\partial t^2 - \Delta$.

Proof Since $\Omega_m(\cdot)$ is invariant under $\mathscr{L}_+^\uparrow$, $U_m(\cdot,\cdot)$ is a continuous unitary representation of $\mathscr{P}_+^\uparrow$ on $L^2(H_m, d\Omega_m)$. By definition, $\Gamma(U)$ is the strongly continuous unitary group $\bigotimes_{k=1}^n U_m(\cdot,\cdot)$ on $\mathscr{H}_s^{(n)}$ for each n. Thus $\Gamma(U_m)$ is a unitary group on $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ and since $\Gamma(U)$ is strongly continuous on F_0, it is strongly continuous on $\mathscr{F}_s$. This verifies that Property 1 holds.

To verify Property 2, we must show that the four-parameter unitary group $\Gamma(U_m(a, I))$ has spectrum with support in the forward light cone. First notice that $L^2(H_m, d\Omega_m)$ is already a spectral representation for $U_m(a, I)$ since $(\eta, U_m(a, I)\eta) = \int_{H_m} e^{ip\cdot\tilde{a}}|\eta(p)|^2\, d\Omega_m(p)$. Since $\Gamma(U_m(a, I)) \restriction \mathscr{H}_s^{(n)} = \bigotimes_{k=1}^n U_m(a, I)$, if $\eta \in \mathscr{H}_s^{(n)}$, and $n > 0$, then

$$(\eta, \Gamma(U_m(a, I))\eta) = \int_{\mathbb{R}^4}\cdots\int_{\mathbb{R}^4} \exp\left(i\left(\sum_{i=1}^n p_i\right)\cdot\tilde{a}\right)|\eta(p_1, \ldots, p_n)|^2 \prod_{i=1}^n d\Omega_m(p_i)$$

$$= \int_{\mathbb{R}^4} e^{i\lambda\cdot\tilde{a}}\, d\mu_\eta(\lambda)$$

where $\mu_\eta(S) = \int\cdots\int_{\sum p_i \in S}|\eta(p_1, \ldots, p_n)|^2 \prod_{i=1}^n d\Omega_m(p_i)$. Since Ω_m has support in $\overline{V}_+$ and $\overline{V}_+$ is a cone, μ_η also has support in $\overline{V}_+$. Now, if $\psi = \{\psi^{(n)}\}_{n=0}^\infty$ is a general vector in $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ and μ_ψ the spectral measure so that

$$(\psi, \Gamma(U_m(a, I))\psi) = \int e^{ip\cdot\hat{a}}\, d\mu_\psi(p)$$

then $\mu_\psi = \sum_{n=0}^\infty \mu_{\psi^{(n)}}$, since $\Gamma(U_m)$: $\mathscr{H}_s^{(n)} \to \mathscr{H}_s^{(n)}$.

The vector $\Omega_0 = \{1, 0, 0, \ldots\}$ is invariant under $\Gamma(U_m(\cdot,\cdot))$ since by definition $\Gamma(U_m)$ acts like the identity on $H_s^{(0)} = \mathbb{C}$. Since no nonzero vector in $L^2(H_m, d\Omega_m)$ is invariant under $U_m(a, I)$ for all $a \in \mathbb{R}^4$, there is no nonzero vector in $\mathscr{H}_s^{(n)}$ which is invariant under $\bigotimes_{k=1}^n U_m(\cdot, I)$. Since $\Gamma(U_m)$: $\mathscr{H}_s^{(n)} \to \mathscr{H}_s^{(n)}$, this implies that the only nonzero invariant vector in $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ is (all scalar multiples of) Ω_0. This verifies Property 3.

Property 4 follows immediately from the definition of Φ_m: $\Phi_m(f) = \Phi_S(Ef)$ for real f and $\Phi_m(f) = \Phi_m(\mathrm{Re}\, f) + i\Phi_m(\mathrm{Im}\, f)$ for complex-valued f, and the fact that $\Phi_S(f)$: $F_0 \to F_0$.

Suppose that $\psi_1, \psi_2 \in F_0$ and $f_n \to f \in \mathscr{S}(\mathbb{R}^n)$ with f_n real-valued. Then

$$Ef_n = \sqrt{2\pi}\, \hat{f}_n \restriction H_m \xrightarrow{L^2(H_m,\, d\Omega_m)} \sqrt{2\pi}\, \hat{f} \restriction H_m = Ef$$

Thus from Theorem X.41d we conclude that

$$(\psi_1, \Phi_m(f_n)\psi_2) \to (\psi_1, \Phi_m(f)\psi_2)$$

By treating the real and imaginary parts of f separately we therefore obtain $(\psi_1, \Phi_m(\cdot)\psi_2) \in \mathscr{S}'(\mathbb{R}^n)$ verifying Property 5.

To prove the Poincaré invariance of the field, notice that $\Gamma(U_m)$: $F_0 \to F_0$ and that if $\psi \in F_0$ and f is a real-valued function in $\mathscr{S}(\mathbb{R}^4)$, then

$$\begin{aligned}\Gamma(U_m(a, \Lambda))\Phi_m(f)\Gamma(U_m(a, \Lambda))^{-1}\psi &= \Gamma(U_m)\Phi_S(Ef)\Gamma(U_m)^{-1}\psi \\ &= \Phi_S(U_m Ef)\psi\end{aligned}$$

by Theorem X.41e. A change of variables shows that $U_m(a, \Lambda)Ef = E(\langle a, \Lambda\rangle f)$, so $\Gamma(U_m(a, \Lambda))\Phi_m(f)\Gamma(U_m(a, \Lambda))^{-1} = \Phi_m(\langle a, \Lambda\rangle f)$. Since both sides of this expression are linear in f and $\Gamma(U_m)$ is a linear operator, the formula is valid for complex-valued f also.

To prove microscopic causality, we must show that for all $f, g \in \mathscr{S}(\mathbb{R}^4)$ with spacelike separated supports and all $\psi \in F_0$,

$$\Phi_m(f)\Phi_m(g)\psi - \Phi_m(g)\Phi_m(f)\psi = 0 \tag{X.69}$$

Since $\Phi_m(\cdot)$ is linear, it is sufficient to prove (X.69) in the case where f and g are real-valued. Then, by (X.64)

$$\begin{aligned}[\Phi_m(f), \Phi_m(g)]\psi &= [\Phi_S(Ef), \Phi_S(Eg)]\psi \\ &= (i\, \mathrm{Im}(Ef, Eg)_{L^2(H_m,\, d\Omega_m)})\psi \\ &= \left(\frac{2\pi}{2}\int_{H_m} (\overline{\hat{f}(p)}\hat{g}(p) - \hat{f}(p)\overline{\hat{g}(p)})\, d\Omega_m(p)\right)\psi \\ &= \left(\int_{\mathbb{R}^4}\int_{\mathbb{R}^4} \frac{1}{2i}\Delta_m(x - y)f(x)g(y)\, dx\, dy\right)\psi\end{aligned}$$

where

$$\Delta_m(x) = \frac{i}{2(2\pi)^3}\int (e^{-i\tilde{p}\cdot x} - e^{ip\cdot x})\, d\Omega_m(p)$$

Now, $\Delta_m(x) = \Delta_+(x; m^2) - \Delta_+(-x; m^2)$, so since $\Delta_+(x; m^2) = f_S(x^2)$ for x spacelike (Theorem IX.48), we conclude that supp $\Delta_m \subset \overline{V}_+ \cup (-\overline{V}_+)$. Thus

$$\iint \Delta_m(x - y)f(x)g(x)\, dx\, dy = 0$$

which implies (X.69).

The cyclicity of the vacuum for $\Phi_m(\cdot)$ follows immediately from Theorem X.41 (parts (b) and (d)) and the fact that the range of the map E on $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^4)$ is dense in $L^2(H_m, d\Omega_m)$ (Problem 44).

Finally, if $f \in \mathscr{S}(\mathbb{R}^4)$, then $\widehat{(\Box^2 + m^2)}f(p) = -(p\cdot\tilde{p} - m^2)\hat{f}(p)$ so

$$E((\Box^2 + m^2)f) = 0$$

Thus $\Phi_m((\Box^2 + m^2)f) = 0$ for all $f \in \mathscr{S}(\mathbb{R}^4)$. ∎

Notice that by the computation above the spectral weight ρ of the Källen–Lehman representation for Φ_m is the point mass at m.

Classical mechanics has provided such a successful framework in physics that it is natural to rephrase physical systems in terms of certain "fixed-time degrees of freedom" which evolve in time. We do this now for the free field by introducing the time-zero field and the canonical conjugate momentum. We emphasize that this choice of a fixed time is not relativistically invariant. As a result, in constructing an interacting field theory by perturbing the free theory using the time-zero fields, it is difficult to recover Lorentz invariance. There is no direct connection between the canonically conjugate momentum and the physical momentum operator P.

We begin in the abstract setting. Recall that a **conjugation** on a Hilbert space $\mathscr{H}$ is an antilinear isometry C so that $C^2 = I$.

Definition Let $\mathscr{H}$ be a complex Hilbert space, $\Phi_S(\cdot)$ the associated Segal quantization. Let C be a conjugation on $\mathscr{H}$ and define $\mathscr{H}_C = \{f \in \mathscr{H} \mid Cf = f\}$. For each $f \in \mathscr{H}_C$ we define $\varphi(f) = \Phi_S(f)$ and $\pi(f) = \Phi_S(if)$. The map $f \mapsto \varphi(f)$ is called the **canonical free field** over $\langle \mathscr{H}, C\rangle$ and the map $f \mapsto \pi(f)$ is called the **canonical conjugate momentum**. We often drop the $\langle \mathscr{H}, C\rangle$ and just write $\mathscr{H}$ if the intended conjugation is clear. Notice that the set of elements of $\mathscr{H}$ for which the maps $f \mapsto \varphi(f)$ and $f \mapsto \pi(f)$ are defined depends on the conjugation C.

Theorem X.43 Let $\mathscr{H}$ be a complex Hilbert space with conjugation C. Let $\varphi(\cdot)$ and $\pi(\cdot)$ be the corresponding canonical fields. Then:

(a) (i) For each $f \in \mathscr{H}_C$, $\varphi(f)$ is essentially self-adjoint on F_0.
(ii) $\{\varphi(f) \mid f \in \mathscr{H}_C\}$ is a commuting family of self-adjoint operators.

(iii) Ω_0 is a cyclic vector for the family $\{\varphi(f) \mid f \in \mathscr{H}_C\}$.

(iv) If $f_n \xrightarrow{\mathscr{H}_C} f$, then

$$\varphi(f_n)\psi \to \varphi(f)\psi \qquad \text{for all } \psi \in F_0$$

and

$$e^{i\varphi(f_n)}\psi \to e^{i\varphi(f)}\psi \qquad \text{for all } \psi \in \mathscr{F}_s(\mathscr{H})$$

(b) Properties (i)–(iv) hold with $\varphi(\cdot)$ replaced by $\pi(\cdot)$.

(c) If $f, g \in \mathscr{H}_C$, then

$$\varphi(f)\pi(g)\psi - \pi(g)\varphi(f)\psi = i(f, g)\psi \qquad \text{for all } \psi \in F_0 \tag{X.70}$$

$$e^{i\varphi(f)}e^{i\pi(g)} = e^{-i(f, g)}e^{i\pi(g)}e^{i\varphi(f)} \tag{X.71}$$

Proof Parts (a)(i) and (a)(iv) follow immediately from the corresponding properties of $\Phi_S(\cdot)$ proven in Theorem X.41. Part (a)(iii) is left to the reader (Problem 43). To see that $\{\varphi(f) \mid f \in \mathscr{H}_C\}$ is a commuting family, notice that (X.65) implies

$$e^{it\varphi(f)}e^{is\varphi(g)} = e^{-its\,\mathrm{Im}(f, g)}e^{is\varphi(g)}e^{it\varphi(f)}$$

where we have used the fact that $\varphi(\cdot)$ is real linear. If $f, g \in \mathscr{H}_C$, then it follows from polarization that $(f, g) = (Cf, Cg) = (g, f)$, so $\mathrm{Im}(f, g) = 0$. Thus $e^{it\varphi(f)}e^{is\varphi(g)} = e^{is\varphi(g)}e^{it\varphi(f)}$ for all s and t. Therefore, by Theorem VIII.13, $\varphi(f)$ and $\varphi(g)$ commute.

The proof of (b) is similar to the proof of (a). (X.70) and (X.71) follow immediately from (X.64), (X.65), and the fact that if $f, g \in \mathscr{H}_C$, then $\mathrm{Im}(f, ig) = \mathrm{Re}(f, g) = (f, g)$. ∎

We now define the conjugation which we will use for the free scalar field of mass m. We write $f \in L^2(H_m, d\Omega_m)$ as $f(p_0, \mathbf{p})$ and define $(Cf)(p_0, \mathbf{p}) = \overline{f(p_0, -\mathbf{p})}$. Notice that C is well-defined on $L^2(H_m, d\Omega_m)$ since $\langle p_0, \mathbf{p}\rangle \in H_m$ if and only if $\langle p_0, -\mathbf{p}\rangle \in H_m$. C is clearly a conjugation. We denote the canonical fields corresponding to C by $\varphi(\cdot)$ and $\pi(\cdot)$ and define

$$\varphi_m(f) = \varphi(Ef)$$
$$\pi_m(f) = \pi(\mu Ef), \qquad \mu = \sqrt{\mathbf{p}^2 + m^2}$$

for real-valued $f \in \mathscr{S}(\mathbb{R}^4)$, extending to all of $\mathscr{S}(\mathbb{R}^4)$ by linearity. In terms of a^-,

$$\varphi_m(f) = \frac{1}{\sqrt{2}}\{(a^-(Ef))^* + a^-(CEf)\}$$

$$\pi_m(f) = \frac{i}{\sqrt{2}}\{(a^-(\mu Ef))^* - a^-(C\mu Ef)\}$$

We warn the reader that the a's in these last formulas differ from those most often used in discussing the free field and that the correct space–time free field is Φ_m and not φ_m; as we will discuss below, φ_m and π_m are useful for discussing the time-zero field. The maps $f \mapsto \varphi_m(f)$ and $f \mapsto \pi_m(f)$ are complex linear and $\varphi_m(f)$, $\pi_m(f)$ are self-adjoint if and only if $Ef \in \mathscr{H}_C$.

Because of the projection E we can extend the class of functions on which $\varphi_m(\cdot)$ and $\pi_m(\cdot)$ are defined to include distributions of the form $\delta(t - t_0)g(x_1, x_2, x_3)$ where $g \in \mathscr{S}(\mathbb{R}^3)$. In particular, if $t_0 = 0$, g is real-valued, and $\hat{g}$ is the ***usual*** Fourier transform on $\mathbb{R}^3$, then

$$(CE\widehat{\delta g})(p_0, \mathbf{p}) = \overline{E\widehat{\delta g}(p_0, -\mathbf{p})} = (2\pi)^{-1/2}\overline{\hat{g}(-\mathbf{p})} = (2\pi)^{-1/2}\hat{g}(\mathbf{p}) = E\widehat{\delta g}$$

Thus $E(\delta g)$ and $\mu E(\delta g)$ are in $\mathscr{H}_C$. Therefore $\varphi_m(\delta g)$ and $\pi_m(\delta g)$ are self-adjoint if $g \in \mathscr{S}(\mathbb{R}^3)$ is real. For obvious reasons, the maps $g \mapsto \varphi_m(\delta g)$, $g \mapsto \pi_m(\delta g)$ are called the **time-zero fields**. From now on we will only use test functions of the form δg in $\varphi_m(\cdot)$ and $\pi_m(\cdot)$ and write $\varphi_m(g)$ and $\pi_m(g)$ if $g \in \mathscr{S}(\mathbb{R}^3)$ instead of $\varphi_m(\delta g)$ and $\pi_m(\delta g)$. If f and g are real-valued functions in $\mathscr{S}(\mathbb{R}^3)$, then (X.70) implies that for $\psi \in F_0$,

$$[\varphi_m(f), \pi_m(g)]\psi = i\int_{H_m} \overline{\hat{f}(p)}\hat{g}(p)\mu(p)\psi\, d\Omega_m(p) \tag{X.72}$$

For convenience and also so that our notation coincides with the standard terminology, we now transfer the fields we have constructed from the Fock space built up from $L^2(H_m, d\Omega_m)$ to the Fock space built up from $L^2(\mathbb{R}^3)$. For notational simplicity, we define for $f \in L^2(H_m, d\Omega_m)$

$$a^\dagger(f) = (a^-(f))^*, \qquad a(f) = a^-(Cf)$$

First notice that each function $f(p) \in L^2(H_m, d\Omega_m)$ is in a natural way a function $f(\mathbf{p}) = f(\mu(\mathbf{p}), \mathbf{p})$ on $\mathbb{R}^3$. For each $f \in L^2(H_m, d\Omega_m)$, we define $(Jf)(\mathbf{p}) = f(\mu(\mathbf{p}), \mathbf{p})/\sqrt{\mu(\mathbf{p})}$. J is a unitary map of $L^2(H_m, d\Omega_m)$ onto $L^2(\mathbb{R}^3)$, so $\Gamma(J)$ is a unitary map of $\mathscr{F}_s(L^2(H_m, d\Omega_m))$ onto $\mathscr{F}_s(L^2(\mathbb{R}^3))$. The annihilation and creation operators on $\mathscr{F}_s(L^2(\mathbb{R}^3))$, $\tilde{a}(\cdot)$, $\tilde{a}^\dagger(\cdot)$, are related to $a(\cdot)$ and $a^\dagger(\cdot)$ by the formulas

$$\tilde{a}\left(\frac{f(\mathbf{p})}{\sqrt{\mu(\mathbf{p})}}\right) = \Gamma(J)a(f)\Gamma(J)^{-1}$$

$$\tilde{a}^\dagger\left(\frac{f(\mathbf{p})}{\sqrt{\mu(\mathbf{p})}}\right) = \Gamma(J)a^\dagger(f)\Gamma(J)^{-1}$$

We use the unitary map $\Gamma(J)$ to carry the Wightman fields over to $\mathscr{F}_s(L^2(\mathbb{R}^3))$ by defining

$$\tilde{\Phi}_m(f) \equiv \Gamma(J)\Phi_m(f)\Gamma(J)^{-1}$$
$$= \frac{1}{\sqrt{2}}\left\{\tilde{a}\left(\tilde{C}\frac{Ef}{\sqrt{\mu}}\right) + \tilde{a}^\dagger\left(\frac{Ef}{\sqrt{\mu}}\right)\right\} \qquad \text{for real-valued } f \in \mathscr{S}(\mathbb{R}^4)$$
$$\tilde{\varphi}_m(f) \equiv \Gamma(J)\varphi_m(f)\Gamma(J)^{-1}$$
$$= \frac{1}{\sqrt{2}}\left\{\tilde{a}\left(\frac{E(f\delta)}{\sqrt{\mu}}\right) + \tilde{a}^\dagger\left(\frac{E(f\delta)}{\sqrt{\mu}}\right)\right\} \qquad \text{for real-valued } f \in \mathscr{S}(\mathbb{R}^3)$$

where $\tilde{C} = JCJ^{-1}$ acts by $(\tilde{C}g)(\mathbf{p}) = \overline{g(-\mathbf{p})}$. *Having established this correspondence, we now drop the* $\sim$ *and the bold face letters;* from now on we will only deal with the fields on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ and three-dimensional momenta. Further, we recall that the restriction of the four-dimensional Fourier transform that we have been using in this section to functions of the form $\delta(x_0)g(x_1, x_2, x_3)$ is the usual three-dimensional Fourier transform. Notice that

$$\check{f} = (\hat{Cf})^{\vee}$$

so $C\hat{f} = \hat{f}$ if and only if f is real-valued.

For f and g real-valued, (X.72) becomes

$$[\varphi_m(f), \pi_m(g)] = i\int f(x)g(x)\,d^3x \tag{X.73}$$

(X.73) is the Schwartz space form of the canonical commutation relations (CCR). In the Appendix to this section we prove that for each $m > 0$, this representation of the CCR is irreducible and for different m, the representations are inequivalent. Thus, the time-zero fields in the free scalar field theories give rise to different representation of the CCR.

As a final topic before turning to interacting fields we will show how the structures which we have developed are related to the "fields" and "annihilation and creation operators" introduced in physics texts. First we let

$$D_{\mathscr{S}} = \{\psi \mid \psi \in F_0, \psi^{(n)} \in \mathscr{S}(\mathbb{R}^{3n}) \text{ for all } n\}$$

and for each $p \in \mathbb{R}^3$ we define an operator $a(p)$ on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ with domain $D_{\mathscr{S}}$ by

$$(a(p)\psi)^{(n)}(k_1, \ldots, k_n) = \sqrt{n+1}\,\psi^{(n+1)}(p, k_1, \ldots, k_n) \tag{X.74}$$

The adjoint of the operator $a(p)$ is *not* a densely defined operator since it is given formally by

$$(a^\dagger(p)\psi)^{(n)}(k_1, \ldots, k_n) = \frac{1}{\sqrt{n}}\sum_{\ell=1}^{n}\delta(p-k_\ell)\psi^{(n-1)}(k_1, \ldots, k_{\ell-1}, k_{\ell+1}, \ldots, k_n) \tag{X.75}$$

However, $a^\dagger(p)$ is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. For example, if $\psi_1 = \{0, \psi^{(1)}, 0, \ldots\}$ and $\psi_2 = \{0, 0, \psi^{(2)}, 0, \ldots\}$, then

$$(\psi_2, a^\dagger(p)\psi_1) = \frac{1}{\sqrt{2}}\int \overline{(\psi^{(2)}(k_1, p)}\psi^{(1)}(k_1) + \overline{\psi^{(2)}(p, k_1)}\psi^{(1)}(k_1))\,dk_1$$

The reader can easily check that the formulas

$$a(g) = \int_{\mathbb{R}^3} a(p)g(-p)\,dp \tag{X.76a}$$

$$a^\dagger(g) = \int_{\mathbb{R}^3} a^\dagger(p)g(p)\,dp \tag{X.76b}$$

hold for all $g \in \mathscr{S}(\mathbb{R}^3)$ if the equalities are understood in the sense of quadratic forms. That is, (X.76a) means that for $\psi_1, \psi_2 \in D_{\mathscr{S}}$, we have

$$(\psi_1, a(g)\psi_2) = \int_{\mathbb{R}^3}(\psi_1, a(p)\psi_2)g(-p)\,dp$$

and similarly for (X.76b). Since $a(p)$: $D_{\mathscr{S}} \to D_{\mathscr{S}}$ the powers of $a(p)$ are well-defined operators on $D_{\mathscr{S}}$. As before we can write down a formal expression for $(a^\dagger(p))^n$, but it does not make sense as an operator, only as a quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. Notice that

$$(\psi_1, (a^\dagger(p))^n\psi_2) = ((a(p))^n\psi_1, \psi_2) \tag{X.77}$$

so for each n, $(a^\dagger(p))^n$ and $a(p)^n$ are "adjoints" in the sense of quadratic forms. We could of course have defined the quadratic form $a^\dagger(p)^n$ by (X.77) and then calculated that it arises by taking the nth power of the formal object given by (X.75). Since $a(p_1)$: $D_{\mathscr{S}} \to D_{\mathscr{S}}$, $(\psi_1, a^\dagger(p_2)a(p_1)\psi_2)$ is a well-defined quadratic form for all $\langle p_1, p_2\rangle \in \mathbb{R}^3 \times \mathbb{R}^3$. Notice, however, that $(\psi_1, a(p_1)a^\dagger(p_2)\psi_2)$ does not make sense since $a^\dagger(p_2)$ is only a quadratic form. In general any product $\prod_{i=1}^{N_1} a(p_i)$ is a well-defined operator from $D_{\mathscr{S}}$ to $D_{\mathscr{S}}$ and $\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)$ is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. Thus

$$\left(\psi_1, \left(\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{N_1} a(p_i)\right)\psi_2\right)$$

is also well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. One can check directly that if $f_i \in \mathscr{S}(\mathbb{R}^3)$, then as quadratic forms

$$\left(\prod_{i=N_1+1}^{N_2} a^\dagger(f_i)\right)\left(\prod_{i=1}^{N_1} a(f_i)\right) = \int_{\mathbb{R}^{3N_2}} \left(\prod_{i=N_1+1}^{N_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{N_1} a(-p_i)\right)\left(\prod_{i=1}^{N_2} f(p_i)\right) dp_1 \cdots dp_{N_2} \quad \text{(X.78)}$$

and

$$N = \int_{\mathbb{R}^3} a^\dagger(p)a(p)\, dp \quad \text{(X.79)}$$

The generator of time translations in the free scalar field theory of mass m is given by

$$H_0 = \int_{\mathbb{R}^3} \mu(p)a^\dagger(p)a(p)\, dp \quad \text{(X.80)}$$

H_0 is called the **free Hamiltonian of mass** m. (X.78), (X.79), and (X.80) involve no formal manipulations, but are mathematical statements about quadratic forms.

Theorem X.44 Let n_1 and n_2 be nonnegative integers and suppose that $W \in L^2(\mathbb{R}^{3(n_1+n_2)})$. Then there is a unique operator T_W on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ so that $D_{\mathscr{S}} \subset D(T_W)$ is a core for T_W and

(a) $$T_W = \int_{\mathbb{R}^{3(n_1+n_2)}} W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})\left(\prod_{i=1}^{n_1} a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2} a(p_i)\right) dk\, dp \quad \text{(X.81)}$$

as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$.

Furthermore,

(b) If m_1 and m_2 are nonnegative integers so that $m_1 + m_2 = n_1 + n_2$, then $(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}$ is a bounded operator with

$$\|(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\| \leq C(m_1, m_2)\|W\|_{L^2}$$

In particular, if $m_1 = n_1$ and $m_2 = n_2$, then

$$\|(1+N)^{-n_1/2}T_W(1+N)^{-n_2/2}\| \leq \|W\|_{L^2}$$

(c) $$T_W^* = \int_{\mathbb{R}^{3(n_1+n_2)}} \overline{W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})}\left(\prod_{i=1}^{n_2} a^\dagger(p_i)\right)\left(\prod_{i=1}^{n_1} a(k_i)\right) dk\, dp$$

as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$.

(d) If $W_n \to W$ in $L^2(\mathbb{R}^{3(n_1+n_2)})$, then $T_{W_n} \to T_W$ strongly on $D_{\mathscr{S}}$.

(e) F_0 is contained in $D(T_W)$ and $D(T_W^*)$, and on vectors in F_0, T_W and T_W^* are given by the explicit formulas

$$(T_W\psi)^{(\ell-n_2+n_1)} = K(\ell, n_1, n_2)S \times \left[\int W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})\psi^{(\ell)}(p_1, \ldots, p_{n_2}, k_{n_1+1}, \ldots, k_{n_1+\ell-n_2})\, dp\right] \quad \text{(X.82a)}$$

$$(T_W\psi)^{(n)} = 0 \qquad \text{if } n < n_1 - n_2$$

$$(T_W^*\psi)^{(\ell-n_1+n_2)} = K(\ell, n_2, n_1)S \times \left[\int \overline{W(k_1, \ldots, k_{n_1}, p_1, \ldots, p_{n_2})}\psi^{\ell}(k_1, \ldots, k_{n_1}, p_{n_2+1}, \ldots, p_{n_2+\ell-n_1})\, dk\right] \quad \text{(X.82b)}$$

$$(T_W^*\psi)^{(n)} = 0 \qquad \text{if } n < n_2 - n_1$$

where S is the symmetrization operator and

$$K(\ell, n_1, n_2) = \left[\frac{\ell!(\ell + n_1 - n_2)!}{((\ell - n_2)!)^2}\right]^{1/2}$$

Proof For vectors in $D_{\mathscr{S}}$, we define $T_W\psi$ by the formula (X.82a). By the Schwarz inequality and the fact that S is a projection,

$$\|(T_W\psi)^{(\ell-n_2+n_1)}\|^2 \leq K(\ell, n_1, n_2)^2\|W\|^2\|\psi^{(\ell)}\|^2$$

If we now define an operator T_W^* on $D_{\mathscr{S}}$ by using the formula in (X.82b), then for all φ and ψ in $D_{\mathscr{S}}$ one easily verifies that

$$(\varphi, T_W\psi) = (T_W^*\varphi, \psi)$$

Thus, T_W is closable and T_W^* is the restriction of the adjoint of T_W to $D_{\mathscr{S}}$. From now on we will use T_W to denote $\overline{T}_W$ and T_W^* to denote the adjoint of T_W. By the definition of T_W, $D_{\mathscr{S}}$ is a core and further, since T_W is bounded on the ℓ-particle vectors in $D_{\mathscr{S}}$, we have $F_0 \subset D(T_W)$. Since the right-hand side of (X.82a) is also bounded on the ℓ-particle vectors, (X.82a) represents T_W on all ℓ-particle vectors. The proof of the statements in (e) about T_W^* are the same.

To prove (b), let $\psi \in D_{\mathscr{S}}$. Then by the above computation

$$\|((1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\psi)^{(\ell-n_2+n_1)}\|^2 \leq \left(\frac{K(\ell, n_1, n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}\right)^2\|W\|^2\|\psi^{(\ell)}\|^2$$

so that

$$\begin{aligned}\|(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}\psi\| &\leq \left(\sup_{\ell<\infty}\frac{K(\ell,n_1,n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}\right)\|W\|\,\|\psi\| \\ &\leq C(m_1,m_2)\|W\|\,\|\psi\|\end{aligned}$$

where

$$C(m_1,m_2)=\sup_{\ell}\frac{K(\ell,n_1,n_2)}{(1+\ell-n_2+n_1)^{m_1/2}(1+\ell)^{m_2/2}}<\infty$$

since $m_1+m_2=n_1+n_2$. In all the sup's only ℓ so that $\ell-n_2+n_1\geq 0$ occur since the other terms are annihilated by the action of T_W. Thus, $(1+N)^{-m_1/2}T_W(1+N)^{-m_2/2}$ extends to a bounded operator on $\mathscr{F}_s(\mathscr{H})$ with norm less than or equal to $C(m_1,m_2)$. If $m_1=n_1$ and $m_2=n_2$, then $C(m_1,m_2)=1$.

To prove (d) we need only note that if $\psi=\{0,\ldots,\psi^{(\ell)},0,\ldots\}\in D_{\mathscr{S}}$ and $W_n\xrightarrow{L^2}W$, then

$$\begin{aligned}\|T_{W_n}\psi-T_W\psi\| &= \|T_{W_n-W}\psi\| \\ &\leq K(\ell,n_1,n_2)\|W_n-W\|\,\|\psi\| \\ &\to 0 \quad \text{as} \quad n\to\infty\end{aligned}$$

Since $D_{\mathscr{S}}$ consists of finite linear combinations of such vectors, we have shown that T_{W_n} converges strongly on $D_{\mathscr{S}}$ to T_W if $W_n\xrightarrow{L^2}W$.

To prove (a) let $\psi_1,\psi_2\in D_{\mathscr{S}}$ with $\psi_1=\{0,\ldots,\psi_1^{(\ell-n_2+n_1)},0,\ldots\}$ and $\psi_2=\{0,\ldots,\psi_2^{(\ell)},0,\ldots\}$. Then, if $W=(\prod_{i=1}^{n_1}f_i(k_i))(\prod_{i=1}^{n_2}g(p_i))$, the definition of the form $(\prod_{i=1}^{n_1}a^\dagger(k_i))(\prod_{i=1}^{n_2}a(p_i))$ shows that

$$\begin{aligned}(\psi_1,T_W\psi_2)=\int W(k_1,\ldots,k_{n_1},p_1,\ldots,p_{n_2}) \\ \times\left(\psi_1,\left(\prod_{i=1}^{n_1}a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2}a(p_i)\right)\psi_2\right)dk\,dp\end{aligned}\tag{X.83}$$

Since both sides of (X.83) are linear in W, the relationship continues to hold for W's that are finite linear combinations of such products. Since

$$\left(\psi_1,\left(\prod_{i=1}^{n_1}a^\dagger(k_i)\right)\left(\prod_{i=1}^{n_2}a(p_i)\right)\psi_2\right)\in L^2(\mathbb{R}^{3(n_1+n_2)})$$

and since (d) holds, both the right- and left-hand sides of (X.83) are continuous linear functionals on $L^2(\mathbb{R}^{3(n_1+n_2)})$. Since they agree on a dense set, they agree everywhere. Finally, (X.83) extends by linearity to all of $D_{\mathscr{S}}\times D_{\mathscr{S}}$. This proves (a); the proof of (c) is similar. ∎

Finally, we note that as quadratic forms on $D_{\mathscr{S}}$ we can express the free scalar field and the time zero fields in terms of $a^\dagger(k)$ and $a(k)$:

$$\Phi_m(x,t)=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}e^{i(\mu(p)t-p\cdot x)}a^\dagger(p)+e^{-i(\mu(p)t-p\cdot x)}a(p)\frac{d^3p}{\sqrt{2\mu(p)}}\tag{X.84}$$

$$\varphi_m(x)=\frac{1}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}(e^{-ip\cdot x}a^\dagger(p)+e^{ip\cdot x}a(p))\frac{d^3p}{\sqrt{2\mu(p)}}\tag{X.85}$$

$$\pi_m(x)=\frac{i}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}(e^{-ip\cdot x}a^\dagger(p)-e^{ip\cdot x}a(p))\sqrt{\frac{\mu(p)}{2}}\,d^3p\tag{X.86}$$

* * *

Before introducing the Hamiltonian approach for constructing a self-interacting scalar boson field in two-dimensional space–time, it is appropriate to make a few general remarks about interacting quantum field theories. At the present time, most of these theories are premathematical in the following sense. Hamiltonians and fields are written down, but no Hilbert space is given on which they are well-defined operators. The matrix elements of the S-operator are then calculated from the fields and Hamiltonian by formal manipulation. These matrix elements are expressed as power series whose coefficients depend on the vacuum expectation values of a related free field theory. Typically, each coefficient of this power series is given by a divergent integral. One formally cancels these infinities by making various input parameters in the theory infinite and then follows a set of prescriptions for extracting the "principal parts" of the resulting difference of divergent integrals; this is called "renormalization." In quantum electrodynamics, these procedures have produced predictions very close to experimental values. However, only slow progress has been made on the mathematical problem of putting these models on a sound foundation. Substantial mathematical results exist in only a few cases and only in space–time dimensions smaller than 4. In only one model (the theory we discuss below is a special case of this model) have all the Wightman axioms been verified (as of 1974). If these cases are a guide, the mathematical resolution of these problems will require advances in diverse areas of functional analysis: self-adjointness questions, perturbation theory, scattering theory, probability theory, spectral analysis, and C^*-algebras.

An "interacting field theory" is a field theory satisfying the Wightman axioms which has a nontrivial scattering theory (see Section XII.15). A

natural way to construct such fields is to try to make a perturbation of one of the free theories which we have constructed. In classical Lagrangian field theory the simplest Hamiltonians are of the form

$$H = H_0 + \int_{\mathbb{R}^3} F(\varphi(x))\, d^3x$$

where F is some function, say a polynomial (see Section X.13). Since we want the Hamiltonian to be bounded below, we expect that the polynomial should be of even order and the coefficient of the highest term positive. The case $F(x) = \alpha x^2$ turns out to have a trivial scattering theory; in fact, the resulting theory is just the free field of mass $m + 2\alpha$. The next simplest case is $F(x) = \lambda x^4$. Thus, we are led to considering the formal Hamiltonian

$$H = H_0 + \lambda \int_{\mathbb{R}^3} (\varphi_m(x))^4\, d^3x, \qquad \lambda > 0 \tag{X.87}$$

where H_0 is the Hamiltonian of the free scalar boson field theory of mass m and $\varphi_m(x)$ is the free field at time zero. One's first naïve hope would be to show that H is self-adjoint and then define the interacting field on Fock space by

$$\Phi(x, t) = e^{iHt}\varphi_m(x)e^{-iHt} \tag{X.88}$$

We will not be able to make sense of (X.87) and (X.88) without serious modifications, but using the commutation relations between φ, π, a, and $a^\dagger$, we can formally compute the differential equation which $\Phi(x, t)$ satisfies (this is just the kind of formal manipulation which we warned the reader against in Section VIII.5):

$$\frac{\partial^2}{\partial t^2}\Phi(x, t) = e^{iHt}(i^2)[H, [H, \varphi_m(x)]]e^{-iHt}$$

$$[H, \varphi_m(x)] = [H_0, \varphi_m(x)]$$

$$= \iint \frac{\mu(k)}{(2\pi)^{3/2}\sqrt{2\mu(\ell)}} \{e^{+ik\cdot x}[a^\dagger(k)a(k), a(\ell)] + e^{-ik\cdot x}[a^\dagger(k)a(k), a^\dagger(\ell)]\}\, dk\, d\ell$$

$$= \iint \frac{\mu(k)}{(2\pi)^{3/2}\sqrt{2\mu(\ell)}} \{e^{+ik\cdot x}(-a(k)\delta(k-\ell)) + e^{-ik\cdot x}a^\dagger(k)\delta(k-\ell)\}\, dk\, d\ell$$

$$= \int \frac{\sqrt{\mu(k)}}{(2\pi)^{3/2}\sqrt{2}}(-e^{+ik\cdot x}a(k) + e^{-ik\cdot x}a^\dagger(k))\, dk = -i\pi_m(x)$$

$$[H, [H, \varphi_m(x)]] = [H_0, [H, \varphi_m(x)]] + [H_I, [H, \varphi_m(x)]]$$

$$[H_0, [H, \varphi_m(x)]] = \int \frac{(\mu(k))^2}{\sqrt{2\mu(k)}\,(2\pi)^{3/2}}(e^{+ik\cdot x}a(k) + e^{-ik\cdot x}a^\dagger(k))\, dk$$

$$= (-\Delta + m^2)\varphi_m$$

$$[\varphi_m(y), [H, \varphi_m(x)]] = \int \frac{e^{-ik\cdot(x-y)}}{(2\pi)^{3/2}}\, d^3k = \delta(x-y)$$

$$[H_I, [H, \varphi_m(x)]] = \lambda \int [\varphi_m(y)^4, [H, \varphi_m(x)]]\, dy$$

$$= 4\lambda \int \varphi_m(y)^3\delta(x-y)\, dy$$

$$= 4\lambda\varphi_m(x)^3$$

Thus,

$$\frac{\partial^2}{\partial t^2}\Phi(x, t) = e^{iHt}(\Delta - m^2)\varphi_m(x)e^{-iHt} - 4\lambda e^{iHt}\varphi_m(x)^3e^{-iHt}$$

$$= (\Delta - m^2)e^{iHt}\varphi_m(x)e^{-iHt} - 4\lambda(e^{iHt}\varphi_m(x)e^{-iHt})^3$$

$$= (\Delta - m^2)\Phi(x, t) - 4\lambda\Phi(x, t)^3$$

Thus, formally the field $\Phi(x, t)$ satisfies

$$(\Box^2 + m^2)\Phi(x, t) = -4\lambda(\Phi(x, t))^3 \tag{X.89}$$

Another way of looking at our problem is that we are trying to find an operator-valued distribution $\Phi(x, t)$ which satisfies (X.89) and also satisfies the Wightman axioms. Henceforth, we write $\varphi(x)$ instead of $\varphi_m(x)$.

We now return to the consideration of (X.87). Although $\varphi(x)$ is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$, it is not an operator, so we must say what we mean by the fourth power $(\varphi(x))^4$. Suppose that we take the expression for $\varphi(x)$ given by (X.85) and formally take the fourth power as if $\varphi(x)$ were an operator. We get a sum of sixteen terms of the form

$$\iiiint_{\mathbb{R}^3\cdots\mathbb{R}^3} \exp\left(-i\sum_{i=1}^4 k_j x\right)\left(\prod_{j=1}^4 (2\pi)^{-3/2}(2\mu(k_j))^{-1/2}\right)\left(\prod_{j=1}^4 a^\#(k_j)\right) dk_1\cdots dk_4 \tag{X.90}$$

where $a^\#(k_j)$ stands for either $a(-k_j)$ or $a^\dagger(k_j)$. As we have already learned, expressions of the form (X.90) do not in general make sense even as quadratic forms unless all the $a^\dagger$ terms are to the left of all the a terms. However,

if all the $a^\dagger$ terms are to the left, then for each x, (X.90) is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. We therefore define the ***n*th Wick power** of $\varphi(x)$ to be the quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$ obtained by formally taking the nth power of $\varphi(x)$ and moving all the $a^\dagger$ terms to the left of the a terms. The nth Wick power of $\varphi(x)$ will be denoted by $:\varphi(x)^n:$. We note that the nth Wick power should really be called the nth Wick power *with respect to* Ω_0 (see Problem 48). The reader can check that *formally*

$$:\varphi(x)^4: = \varphi(x)^4 - c\varphi(x)^2 + d$$

where c and d are appropriately chosen infinite constants. By putting in cut-offs we will later make precise mathematical sense out of this statement.

If we now replace $(\varphi(x))^4$ by $:\varphi(x)^4:$ in (X.87), then H is a well-defined quadratic form on $D_{\mathscr{S}} \times D_{\mathscr{S}}$. For example, if $\psi_i = \{0, 0, 0, \psi_i^{(3)}, 0, \ldots\}$, $i = 1, 2$, then the term in $(\psi_1, H\psi_2)$ with two $a^\dagger$'s and two a's is

$$\int \left(\iiiint \left(\frac{\exp(-ix(k_1 + k_2 - k_3 - k_4))}{\prod_{j=1}^4 (2\mu(k_j))^{1/2}(2\pi)^{3/2}} \right) \times \left(\iint \overline{\psi_1^{(3)}(p_1, k_1, k_2)} \psi_2^{(3)}(p_2, k_3, k_4)\, dp_1\, dp_2 \right) dk_1 \cdots dk_4 \right) dx \quad \text{(X.91)}$$

This is a well-defined finite integral since $\psi_i^{(3)} \in \mathscr{S}(\mathbb{R}^3)$. Unfortunately, this quadratic form does not arise from an operator. To see this, consider the formal expression for $H\Omega_0$. This is a vector $(0, 0, 0, 0, \psi^{(4)}, 0, \ldots)$ with (formally)

$$\psi^{(4)}(k_1, k_2, k_3, k_4) = \int_{\mathbb{R}^3} \frac{\exp(-ix \sum_{i=1}^4 k_i)}{\prod_{i=1}^4 (2\pi)^{3/2}(2\mu(k_i))^{1/2}}\, dx = \frac{\delta(\sum_{i=1}^4 k_i)}{(2\pi)^{9/2} \prod_{i=1}^4 (2\mu(k_i))^{1/2}}$$

This expression is certainly not in $L^2(\mathbb{R}^{(3)(4)})$; first, of course, it is singular because of the delta function, but even if we restrict the x integration by letting $g \in C_0^\infty(\mathbb{R}^3)$ and consider

$$\int \frac{g(x)\exp(-ix \sum_{i=1}^4 k_i)}{\prod_{i=1}^4 (2\pi)^{3/2}(2\mu(k_i))^{1/2}}\, dx = \frac{\hat{g}(\sum_{i=1}^4 k_i)}{(2\pi)^{9/2} \prod_{i=1}^4 (2\mu(k_i))^{1/2}}$$

we still do not get an L^2 function because $\mu(k_i)$ grows too slowly at ∞. Thus, there are two kinds of infinities involved here: the infinite volume (x space) divergence and the ultraviolet (large k) divergence.

In order to obtain an operator, we *restrict ourselves to one space dimension* (i.e., each of the k_i, p_i, and x are now one dimensional) and replace the quadratic form $\int_{\mathbb{R}} :\varphi(x)^4: dx$ by $\int_{\mathbb{R}} g(x):\varphi(x)^4: dx$ where $g(x)$ is a real-valued function in $L^2(\mathbb{R})$. Then, each of the terms in the quadratic form

$$H_0 + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

has a kernel of the form $\hat{g}(\sum_{j=1}^4 k_j)/\prod_{j=1}^4 (2\mu(k_j))^{1/2}$. Since this function is in $L^2(\mathbb{R}^4)$ (Problem 47), we are guaranteed by Theorem X.44 that the quadratic form arises from an operator on $D_{\mathscr{S}}$ which is symmetric since g is real-valued. We denote by $H_I(g)$ the operator $\int_{\mathbb{R}} g(x):\varphi(x)^4: dx$ and define on $D_{\mathscr{S}}$

$$H(g) = H_0 + H_I(g) = H_0 + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

We will often choose for g a smooth function of compact support which equals one on a very large interval. Occasionally, one takes the characteristic function of a large interval for g. In either case, the effect of g is to turn off the interaction for large values of x. Therefore, g is called a **space cut-off** and $H(g)$ is called the **spatially cut-off Hamiltonian for the $(\varphi^4)_2$ field theory** (the 2 refers to the fact that we are using only one space dimension, so space–time is two dimensional). We summarize in a proposition.

Proposition Let φ be the free scalar boson field of mass m at $t = 0$ in two-dimensional space–time. Let g be a real-valued function in $L^2(\mathbb{R})$. Then

$$H(g) = H_0 + H_I(g) = \int_{\mathbb{R}} \mu(k)a^\dagger(k)a(k)\, dk + \int_{\mathbb{R}} g(x):\varphi(x)^4: dx$$

is a well-defined symmetric operator on $D_{\mathscr{S}}$.

In Section 9 we will show that $H(g)$ is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$. In Chapter XIX we will show how von Neumann algebras can be used to remove the spatial cut-off by choosing a new representation of the canonical commutation relations.

The procedure that we have just indicated for controlling the infinite volume infinity by putting in a spatial cut-off which is then removed by C^*-algebra techniques is generally believed to be the correct method for handling this infinity in more general quantum field theories. It is thought that the ultraviolet divergences in $(\varphi^4)_3$ and $(\varphi^4)_4$ can be removed by a procedure known as renormalization together with a change of representation of the commutation relations. To describe renormalization very briefly recall that we have seen that the Wick ordering of powers of the

field can be interpreted as subtracting a lower order polynomial with infinite coefficients. In $(\varphi^4)_3$ it is known, and in $(\varphi^4)_4$ it is expected, that a similar procedure of subtracting terms with infinite constants will work except that the constants will no longer be linear in λ as they are for Wick ordering. For further discussion and references to the $(\varphi^4)_3$ results, see the Notes.

Our final topic is the construction of **Q-space** and $L^2(Q, d\mu)$, another representation of the Fock space structures which we have presented. In analogy with the one degree of freedom case where $\mathscr{F}(\mathbb{R})$ is isomorphic to $L^2(\mathbb{R}, dx)$ in such a way that $\Phi_S(1)$ becomes multiplication by x, we will construct a measure space $\langle Q, \mu\rangle$, with $\mu(Q) = 1$, and a unitary map S: $\mathscr{F}_s(\mathscr{H}) \to L^2(Q, d\mu)$ so that for each $f \in \mathscr{H}_C$, $S\varphi(f)S^{-1}$ acts on $L^2(Q, d\mu)$ by multiplication by a measurable function. We can then show that in the case of the free scalar field of mass m in two-dimensional space–time, $V \equiv SH_I(g)S^{-1}$ is just multiplication by a function $V(q)$ which is in $L^p(Q, d\mu)$ for each $p < \infty$. In Section X.9, we will use this property of V in a proof that $H = H_0 + H_I(g)$ is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$.

Let $\{f_n\}_{n=1}^\infty$ be an orthonormal basis for $\mathscr{H}$ so that each $f_n \in \mathscr{H}_C$ and let $\{g_k\}_{k=1}^N$ be a finite collection of the f_n. Let $\mathscr{F}_N$ be the closure of the set

$$\{P(\varphi(g_1), \ldots, \varphi(g_N))\Omega_0 \,|\, P \text{ a polynomial}\}$$

in $\mathscr{F}_s(\mathscr{H})$ and define $F_0^{(N)} = \mathscr{F}_N \cap F_0$. From Theorem X.43 (and its proof) it follows that $\varphi(g_k)$ and $\pi(g_\ell)$ are essentially self-adjoint on $F_0^{(N)}$ and that

$$e^{it\varphi(g_k)}e^{is\pi(g_\ell)} = e^{-ist\delta_{k\ell}}e^{is\pi(g_\ell)}e^{it\varphi(g_k)}$$

Thus we have a representation of the Weyl relations in which the vector Ω_0 satisfies $(\varphi(g_k)^2 + \pi(g_k)^2 - 1)\Omega_0 = 0$ and is cyclic for the operators $\{\varphi(g_k)\}_{k=1}^N$. Therefore by the construction in Problem 30 (or we could appeal directly to Theorem VIII.14), there is a unitary map $\tilde{S}^{(N)}$: $\mathscr{F}_N \to L^2(\mathbb{R}^N)$ so that

$$\tilde{S}^{(N)}\varphi(g_k)(\tilde{S}^{(N)})^{-1} = x_k$$

$$\tilde{S}^{(N)}\pi(g_k)(\tilde{S}^{(N)})^{-1} = \frac{1}{i}\frac{d}{dx}$$

and

$$\tilde{S}^{(N)}\Omega_0 = \pi^{-N/4}\exp\left(-\sum_{k=1}^N \frac{x_k^2}{2}\right)$$

It is convenient to use the Hilbert space $L^2(\mathbb{R}^N, \pi^{-N/2}\exp(-\sum_{k=1}^N x_k^2)\,d^Nx)$ instead of $L^2(\mathbb{R}^N)$ so let $d\mu_k = \pi^{-1/2}e^{-x_k^2}\,dx_k$ and define $(Tf)(x) = \pi^{N/4}\exp(\sum_{k=1}^N x_k^2/2)f(x)$. Then T is a unitary map of $L^2(\mathbb{R}^N)$ onto

$L^2(\mathbb{R}^N, \prod_{k=1}^N d\mu_k)$ and if we let $S^{(N)} = T\tilde{S}^{(N)}$, we have

$$S^{(N)}\colon \mathscr{F}_N \to L^2\left(\mathbb{R}^N, \prod_{k=1}^N d\mu_k\right)$$

$$S^{(N)}\varphi(g_k)(S^{(N)})^{-1} = x_k$$

$$S^{(N)}\pi(g_k)(S^{(N)})^{-1} = -\frac{x_k}{i} + \frac{1}{i}\frac{\partial}{\partial x_k}$$

$$S^{(N)}\Omega_0 = 1 \qquad \text{(the function identically one)}$$

Notice that each μ_k has mass one, which implies that

$$(\Omega_0, P_1(\varphi(g_1))\cdots P_N(\varphi(g_N))\Omega_0) = \int_{\mathbb{R}^N} P_1(x_1)\cdots P_N(x_N)\prod_{k=1}^N d\mu_k$$

$$= \prod_{k=1}^N \int_{\mathbb{R}} P_k(x_k)\,d\mu_k$$

$$= \prod_{k=1}^N (\Omega_0, P_k(\varphi(g_k))\Omega_0) \qquad \text{(X.92)}$$

where $P_1, \ldots, P_N$ are polynomials. This formula can also be proven, of course, by direct computations on $\mathscr{F}_s(\mathscr{H})$.

Now it is easy to see how to construct $\langle Q, d\mu\rangle$. We define $Q = \times_{k=1}^\infty \mathbb{R}$. Take the σ-algebra generated by countable products of measurable sets in $\mathbb{R}$ and set $\mu = \otimes_{k=1}^\infty \mu_k$. We denote the points of Q by $q = \langle q_1, q_2, \ldots\rangle$. Then $\langle Q, \mu\rangle$ is a measure space and the set of functions of the form $P(q_1, \ldots, q_n)$, where P is a polynomial and n is arbitrary, is dense in $L^2(Q, d\mu)$. For a discussion of the measure-theoretic details, see the references in the Notes. Let P be a polynomial in N variables

$$P(x_{k_1}, \ldots, x_{k_N}) = \sum_{\ell_1, \ldots, \ell_M} c_{\ell_1, \ldots, \ell_N} x_{k_1}^{\ell_1}, \ldots, x_{k_N}^{\ell_N}$$

and define

$$S\colon P(\varphi(f_{k_1}), \ldots, \varphi(f_{k_N}))\Omega_0 \to P(q_{k_1}, \ldots, q_{k_N})$$

Then

$$\|P(\varphi(f_{k_1}), \ldots, \varphi(f_{k_N}))\Omega_0\|^2 = \sum_{\ell, \mathbf{m}} c_\ell\,\bar{c}_{\mathbf{m}}(\Omega_0, \varphi(f_{k_1})^{\ell_1+m_1}\cdots\varphi(f_{k_N})^{\ell_N+m_N}\Omega_0)$$

$$= \sum_{\ell, \mathbf{m}} c_\ell\,\bar{c}_{\mathbf{m}}\int_{\mathbb{R}^N} q_{k_1}^{\ell_1+m_1}\cdots q_{k_N}^{\ell_N+m_N}\prod_{i=1}^N d\mu_{k_i}$$

$$= \int_Q |P(q_{k_1}, \ldots, q_{k_N})|^2\,d\mu$$

by (X.92) and the fact that each μ_k has mass one. Since Ω_0 is cyclic for polynomials in the fields (Theorem X.42), S extends to a unitary map of $\mathscr{F}_s(\mathscr{H})$ onto $L^2(Q, d\mu)$. Clearly $S\varphi(f_k)S^{-1} = q_k$ and $S\Omega_0 = 1$.

Theorem X.45 Let φ_m be the free scalar field of mass m (in two-dimensional space–time) at time zero. Let $g \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ and define

$$H_I(g) = \int_{\mathbb{R}} g(x) :\varphi_m(x)^4: \, dx$$

Let S denote the unitary map of $\mathscr{F}_s(L^2(\mathbb{R}))$ onto $L^2(Q, d\mu)$ constructed above. Then $V \equiv SH_I(g)S^{-1}$ is multiplication by a function $V(q)$ which satisfies:

(a) $V \in L^p(Q, d\mu)$ for all $p < \infty$.
(b) $e^{-tV} \in L^1(Q, d\mu)$ for all $t \in [0, \infty)$.

Proof We will prove (a). See the Notes for a reference for the proof of (b). Let $\chi_n(x)$ be the characteristic function of $(-n, n)$ and define

$$\varphi_m(x, n) = \frac{1}{\sqrt{4\pi}} \int (e^{-ik\cdot x}a(k) + e^{ik\cdot x}a^\dagger(k)) \frac{\chi_n(k)}{\sqrt{\mu(k)}} \, dk$$

Then $\varphi_m(x, n)$ is a well-defined operator-valued *function* of x. We define $:\varphi_m(x, n)^4:$ by moving all the $a^\dagger$'s to the left in the formal expression for $\varphi_m(x, n)^4$. $:\varphi_m(x, n)^4:$ is also a well-defined operator for each x and $:\varphi(x, n)^4:$ takes F_0 into itself. Now define

$$H_I(g, n) = \int_{\mathbb{R}} g(x) :\varphi_m(x, n)^4: \, dx$$

and set $V_n = SH_I(g, n)S^{-1}$. For each x,

$$:\varphi_m(x, n)^4: = \varphi_m(x, n)^4 + d_2(n)\varphi_m(x, n)^2 + d_0(n)$$

where the coefficients d_2 and d_0 are independent of x but dependent on n (Problem 48). For each x, $S\varphi_m(x, n)S^{-1}$ is just the operator on $L^2(Q, d\mu)$ which operates by multiplying by $\sum_{k=1}^{\infty} c_k(x, n)q_k$ where $c_k(x, n) = (2\pi)^{-1/2} \times (f_k, \chi_n \mu^{-1/2} e^{ikx})$. Furthermore, $\sum_{k=1}^{\infty} |c_k(x, n)|^2 = (2\pi)^{-1} \|\chi_n \mu^{-1/2}\|_2^2$, so $S\varphi_m(x, n)^4 S^{-1}$ and $S\varphi_m(x, n)^2 S^{-1}$ are in $L^2(Q, d\mu)$ and the $L^2(Q, d\mu)$ norms are uniformly bounded in x. Therefore, since $g \in L^1(\mathbb{R})$, $SH_1(g, n)S^{-1}$ operates on $L^2(Q, d\mu)$ by multiplication by an $L^2(Q, d\mu)$ function which we denote by $V_n(q)$.

For each n, $H_I(g, n)$ differs from $H_I(g)$ only in that the kernel in each of the terms is $g(\sum k_i) \prod_{i=1}^4 \mu(k_i)^{-1/2} \chi_n(k_i)$. As $n \to \infty$, these kernels converge to $g(\sum k_i) \prod_{i=1}^4 \mu(k_i)^{-1/2}$ in $L^2(\mathbb{R}^4)$. Therefore, by Theorem X.44, $H_I(g, n)\psi \to H_I(g)\psi$ for $\psi \in F_0$. In particular $H_I(g, n)\Omega_0 \to H_I(g)\Omega_0$. But, since $S\Omega_0 = 1$, $\|H_I(g, n)\Omega_0\| = \|SH_I(g, n)S^{-1}\|_{L^2(Q, d\mu)} = \|V_n\|_{L^2(Q, d\mu)}$. Thus, the sequence of functions V_n is Cauchy in $L^2(Q, d\mu)$ and so converges to a function $V \in L^2(Q, d\mu)$. The reader can now easily complete the proof by showing that each $P(q_1, \ldots, q_n)$ is in the domain of V and $SH_I(g)S^{-1} = V$ on that domain. Since Ω_0 is in the domain of $H_I(g)^n$ for all n, 1 is in the domain of V^n for all n. Thus, for all n, $V \in L^{2n}(Q, d\mu)$. Since $\mu(Q) < \infty$, $V \in L^p(Q, d\mu)$ for all $p < \infty$. ∎

Appendix to X.7 The Weyl relations for the free field

In this appendix, we study the natural generalizations of the Weyl relations (VIII.8) to the case of infinitely many degrees of freedom. Let $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ denote the Schwarz space of real-valued functions on $\mathbb{R}^\nu$. Suppose that $f \mapsto U(f)$ and $f \mapsto V(f)$ are maps of $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ into the bounded operators on a separable Hilbert space $\mathscr{H}$ which satisfy:

(i) for each $f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$, $V(f)$ and $U(f)$ are unitary;
(ii) for all $f, g \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$, $V(f)$ and $U(f)$ satisfy

$$V(f+g) = V(f)V(g), \qquad U(f+g) = U(f)U(g) \tag{X.93}$$

$$V(f)U(g) = U(g)V(f)\exp\left(-i\int_{\mathbb{R}^\nu} f(x)g(x)\,dx\right) \tag{X.94}$$

(iii) if $f_n \xrightarrow{\mathscr{S}(\mathbb{R}^\nu)} f$, then $U(f_n) \to U(f)$ and $V(f_n) \to V(f)$ strongly on $\mathscr{H}$.

The pair of maps $\{U(\cdot), V(\cdot)\}$ is called a representation of the **Weyl relations** over $\mathscr{S}(\mathbb{R}^\nu)$. Two such representations, $\{U_1(\cdot), V_1(\cdot)\}$ on $\mathscr{H}_1$ and $\{U_2(\cdot), V_2(\cdot)\}$ on $\mathscr{H}_2$, are called **equivalent** if there is a unitary operator $T: \mathscr{H}_1 \to \mathscr{H}_2$, so that $U_2(f) = TU_1(f)T^{-1}$ and $V_2(f) = TV_1(f)T^{-1}$ for all $f \in \mathscr{S}(\mathbb{R}^\nu)$. The relation (X.71) shows that for each m, the pair $\{e^{i\pi_m(\cdot)}, e^{i\varphi_m(\cdot)}\}$, where π_m, φ_m are the time-zero field and conjugate momentum of the free scalar field of mass m, is a representation of the Weyl relations on $\mathscr{F}_s(L^2(\mathbb{R}^3))$. We will see below that these representations are inequivalent.

Let $\{U(\cdot), V(\cdot)\}$ be a representation of the Weyl relations over $\mathscr{S}(\mathbb{R}^\nu)$ and let $\{h_n\}_{n=1}^\infty$ be the orthonormal basis for $L^2(\mathbb{R}^\nu)$ made up of products of Hermite functions. If $U_n(t) = U(th_n)$ and $V_n(t) = V(th_n)$, then (X.93), (X.94), and (iii) imply that for each n, $U_n(t)$ and $V_n(t)$ are strongly continuous unitary groups on $\mathscr{H}$ that satisfy

$$\begin{aligned} &V_n(t)U_m(s) = U_m(s)V_n(t), \qquad m \neq n \\ &V_n(t)U_m(s) = e^{-ist}U_m(s)V_m(t) \end{aligned} \tag{X.95}$$

for all s, $t \in \mathbb{R}$. Thus, for all n, $\{U_n(t), V_n(s)\}$ satisfy the Weyl relations (VIII.8), and for different n the corresponding unitary operators commute. Von Neumann's theorem (Theorem VIII.14, see Problem 30 and Chapter XIV) states that up to multiplicity, there is only one representation (the Schrödinger representation) of the relations (X.95) if n ranges over a finite set of integers. It was thought for a long time that von Neumann's theorem held for the case of infinitely many n, but examples of inequivalent representations occurred in the work of Friedrichs in the late 1940's and were emphasized in the later work of Segal and Gårding–Wightman. As we have already mentioned, Theorem X.46 below shows that the free scalar fields of different masses give rise to inequivalent representations.

By (X.93) and (iii), $V(tf)$ and $U(tf)$ are continuous unitary groups on $\mathscr{H}$; we denote their generators by $\varphi(f)$ and $\pi(f)$ respectively. It can be shown that there is a domain D in $\mathscr{H}$ which is invariant under all of the operators $\varphi(f), \pi(f), f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^\nu)$ and on which $\varphi(f)$ and $\pi(f)$ are essentially self-adjoint. For $\psi \in D$, (X.94) implies that

$$[\varphi(f), \pi(g)]\psi = i \int_{\mathbb{R}^\nu} f(x)g(x)\, dx\, \psi \tag{X.96}$$

for all f, $g \in \mathscr{S}(\mathbb{R}^\nu)$. A pair of operator-valued distributions over $\mathscr{S}(\mathbb{R}^\nu)$ which satisfy (X.96) are said to be a representation of the **canonical commutation relations**. In the case of the time-zero free scalar field of mass m, we have already seen that D can be chosen to be D_0 and that (X.96) can be verified directly. As in the case of finitely many p_i and q_i discussed in Section VIII.5, (X.96) does not necessarily imply (X.94) although they are formally equivalent.

We now prove that the representations of the canonical commutation relations arising from free scalar fields of different masses $m > 0$ are inequivalent. A family of bounded operators on a Hilbert space is called **irreducible** if the only operators that commute with all members of the family are scalar multiples of the identity.

Lemma 1 Let $\Phi_S(\cdot)$, be the Segal quantization over a separable Hilbert space $\mathscr{H}$. Then the family of operators $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}$ is irreducible.

Proof Let $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ denote the set of operators which commute with all $e^{i\Phi_S(f)}, f \in \mathscr{H}$. Since $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ is a norm closed algebra of operators closed under taking adjoints, the same proof as in the lemma after Theorem VI.19 shows that each operator in $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$ may be written as a linear combination of four unitaries in $\{e^{i\Phi_S(f)} \mid f \in \mathscr{H}\}'$. It is therefore sufficient to prove that every unitary $T \in \{e^{i\Phi(f)} \mid f \in \mathscr{H}\}'$ is a scalar multiple of the identity.

For each $f \in \mathscr{H}$ and all t, T commutes with $e^{it\Phi_S(f)}$ so by Theorem VIII.13, T commutes with the spectral projections of $\Phi_S(f)$. Thus, T: $D(\Phi_S(f)) \to D(\Phi_S(f))$ and $T\Phi_S(f)\psi = \Phi_S(f)T\psi$ for all $\psi \in D(\Phi_S(f))$. Now, let C be a conjugation on $\mathscr{H}$ and for $f \in \mathscr{H}_C$ define $N(f) = \frac{1}{2}(\Phi_S(f)^2 + \Phi_S(if)^2 - 1)$. Then $N(f) \geq 0$, since $N(f) = d\Gamma((f, \cdot)f)$ and T: $D(N(f)) \to D(N(f))$ with $TN(f)\psi = N(f)T\psi$ for $\psi \in D(N(f))$. Let $\{f_i\}_{i=1}^\infty$ be an orthonormal basis for $\mathscr{H}$ with $f_i \in \mathscr{H}_C$ for each i. The reader can check directly that for each $\psi \in D(N)$

$$N\psi = \lim_{n\to\infty} \sum_{i=1}^{n} N(f_i)\psi$$

Thus, $\psi \in Q(N)$, the form domain of N, if and only if $\psi \in \bigcap_{i=1}^\infty Q(N(f_i))$ and $\sum_{i=1}^\infty (\psi, N(f_i)\psi) < \infty$, and if the sum is finite,

$$(\psi, N\psi) = \sum_{i=1}^{\infty} (\psi, N(f_i)\psi)$$

Since $\Omega_0 \in D(N(f_i))$, $T\Omega_0 \in D(N(f_i))$. Thus, since $N(f_i)\Omega_0 = 0$ for all i we have

$$\sum_{i=1}^{\infty} (T\Omega_0, N(f_i)T\Omega_0) = \sum_{i=1}^{\infty} (T^*T\Omega_0, N(f_i)\Omega_0) = 0$$

Therefore, $T\Omega_0 \in Q(N)$ and $(T\Omega_0, NT\Omega_0) = 0$. Since N is strictly positive on $\{\Omega_0\}^\perp$, there exists a constant c so that $T\Omega_0 = c\Omega_0$. Let $\mathscr{P}$ be a polynomial in $\Phi_S(g_1), \ldots, \Phi_S(g_n)$ for some $g_i \in \mathscr{H}$. Then $T(\mathscr{P}\Omega_0) = \mathscr{P}(T\Omega_0) = c\mathscr{P}\Omega_0$. The set of such vectors $\mathscr{P}\Omega_0$ is dense in $\mathscr{F}_s(\mathscr{H})$ by Theorem X.41. Therefore $T = cI$. ∎

Lemma 2 Let $\varphi_m(\cdot)$, $\pi_m(\cdot)$ be the time-zero field and conjugate momentum of the free scalar field of mass m. Then the set

$$\{e^{i\varphi_m(f)}, e^{i\pi_m(f)} \mid f \in \mathscr{S}_{\mathbb{R}}(\mathbb{R}^3)\}$$

is irreducible.

Proof The reader can easily deduce Lemma 2 from Lemma 1 by using the fact that $\mathscr{S}_{\mathbb{R}}(\mathbb{R}^3)$ is dense in $L^2_{\mathbb{R}}(\mathbb{R}^3)$ and the continuity properties of the fields (Theorem X.41d). ∎

Theorem X.46 Let $\varphi_m(\cdot)$, $\pi_m(\cdot)$ be the time-zero field and conjugate momentum of the free scalar field of mass m. Then, if $m_1 \neq m_2$, the representations $\{\exp(i\pi_{m_1}(\cdot)), \exp(i\varphi_{m_1}(\cdot))\}$ and $\{\exp(i\pi_{m_2}(\cdot)), \exp(i\varphi_{m_2}(\cdot))\}$ of the Weyl relations are inequivalent.

Proof Suppose that there exists a unitary map T on $\mathscr{F}_s(L^2(\mathbb{R}^3))$ which satisfies $T\exp(i\varphi_{m_1}(f))T^{-1} = \exp(i\varphi_{m_2}(f))$ and $T\exp(i\pi_{m_2}(f))T^{-1} = \exp(i\pi_{m_1}(f))$ for all $f \in \mathscr{S}(\mathbb{R}^3)$. Let $G_{m_1}(\cdot, \cdot)$ and $G_{m_2}(\cdot, \cdot)$ denote the restrictions of the representations $\Gamma(U_{m_2}(\cdot, \cdot))$ and $\Gamma(U_{m_1}(\cdot, \cdot))$ to the Euclidean group, which is the subgroup of $\mathscr{P}_+^\uparrow$ which leaves the time-zero plane fixed (the semidirect product of the rotation group and the translation group on $\mathbb{R}^3$). For any element $\langle R, a\rangle$ of the Euclidean group, the Poincaré invariance of the fields implies that

$$G_{m_1}(R, a)\varphi_{m_1}(f)G_{m_1}(R, a)^{-1} = \varphi_{m_1}(\langle R, a\rangle f)$$
$$G_{m_2}(R, a)\varphi_{m_2}(f)G_{m_2}(R, a)^{-1} = \varphi_{m_2}(\langle R, a\rangle f)$$

and also the corresponding statements for π_{m_1} and π_{m_2}. From the functional calculus it follows that

$$G_{m_1}(R, a)\exp(i\varphi_{m_1}(f))G_{m_1}(R, a)^{-1} = \exp(i\varphi_{m_1}(\langle R, a\rangle f))$$
$$G_{m_2}(R, a)\exp(i\varphi_{m_2}(f))G_{m_2}(R, a)^{-1} = \exp(i\varphi_{m_2}(\langle R, a\rangle f))$$

and similar statements for π_{m_1} and π_{m_2}. From these relations and the properties of T the reader can quickly check that for each $\langle R, a\rangle$ and each $f \in \mathscr{S}(\mathbb{R}^3)$, $TG_{m_1}(R, a)T^{-1}G_{m_2}(\langle R, a\rangle^{-1})$ commutes with both $\exp(i\pi_{m_2}(f))$ and $\exp(i\varphi_{m_2}(f))$. By Lemma 2 this implies that

$$TG_{m_1}(R, a)T^{-1}G_{m_2}(\langle R, a\rangle^{-1}) = C(R, a)$$

or equivalently

$$TG_{m_1}(R, a)T^{-1} = C(R, a)G_{m_2}(R, a)$$

where $C(R, a)$ is a constant which a priori might depend on R and a. It follows from the above relations that $C(\cdot, \cdot)$ is a one-dimensional representation of the Euclidean group. It is not hard to show (Problem 41) that the identity representation is the only such representation. Thus

$$TG_{m_1}(R, a)T^{-1} = G_{m_2}(R, a)$$

for all $\langle R, a\rangle$ in the Euclidean group. And from this it follows that $T\Omega_0 = \alpha\Omega_0$ since Ω_0 is the unique vector invariant under both G_{m_1} and G_{m_2}. Thus

$$(\Omega_0, \varphi_{m_1}(f)\varphi_{m_1}(g)\Omega_0) = (\Omega_0, T\varphi_{m_1}(f)T^{-1}T\varphi_{m_1}(g)T^{-1}\Omega_0)$$
$$= (\Omega_0, \varphi_{m_2}(f)\varphi_{m_2}(g)\Omega_0)$$

which implies that $(\Omega_0, \varphi_{m_1}(x)\varphi_{m_1}(y)\Omega_0)$ and $(\Omega_0, \varphi_{m_2}(x)\varphi_{m_2}(y)\Omega_0)$ are equal as tempered distributions on $\mathscr{S}(\mathbb{R}^3) \times \mathscr{S}(\mathbb{R}^3)$. But

$$(\Omega_0, \varphi_{m_1}(x)\varphi_{m_1}(y)\Omega_0) = \Delta_+(x - y, m_1^2)$$

and

$$(\Omega_0, \varphi_{m_2}(x)\varphi_{m_2}(y)\Omega_0) = \Delta_+(x - y, m_2^2)$$

and these distributions are *not* equal if $m_1 \neq m_2$. Thus no such T having the indicated properties can exist. Therefore the representations of the Weyl relations are inequivalent. ∎

X.8 Semigroups and their generators

A family of bounded operators $\{T(t) | 0 \leq t < \infty\}$ on a Banach space X is called a **strongly continuous semigroup** if:

(a) $T(0) = I$
(b) $T(s)T(t) = T(s + t)$ for all $s, t \in \mathbb{R}^+$
(c) For each $\varphi \in X$, $t \mapsto T(t)\varphi$ is continuous.

Such semigroups arise naturally in the theory of partial differential equations and in quantum theory; this section is devoted to studying their fundamental properties. We will see that strongly continuous semigroups are the "exponentials," $T(t) = e^{-tA}$, of a certain class of operators. Thus, they provide a generalization of the relationship between unitary groups and self-adjoint operators. In particular, Stone's theorem, the fundamental criterion, the core theorem (Theorem VIII.11), and the Kato–Rellich theorem, all have generalizations to strongly continuous semigroups and their generators. The only important property of self-adjoint operators that does not generalize is the spectral theorem. There is a different class of operators called "spectral operators" for which there is an analogue of the spectral theorem. We give references in the Notes. The theory of semigroups has applications to the study of parabolic and hyperbolic partial differential equations. Throughout this section we use the heat equation to illustrate these applications. More general differential equations are discussed in the Notes.

We begin by studying a special class of semigroups:

Definition A family $\{T(t) | 0 \leq t < \infty\}$ of bounded operators on a Banach space X is called a **contraction semigroup** if it is a strongly continuous semigroup and moreover $\|T(t)\| \leq 1$ for all $t \in [0, \infty)$.

As the reader will see, theorems about general strongly continuous semigroups are easy generalizations of the corresponding theorems for contraction semigroups. Thus, we study the special case first. We then briefly discuss the general theory and conclude the section by studying another special class, holomorphic semigroups.

Let $T(t)$ be a contraction semigroup on a Banach space X. As in the case of unitary groups on Hilbert spaces we obtain the generator of $T(t)$ by differentiation. Set $A_t = t^{-1}(I - T(t))$ and define

$$D(A) = \left\{ \varphi \,\middle|\, \lim_{t \downarrow 0} A_t \varphi \text{ exists} \right\}$$

For $\varphi \in D(A)$, we define $A\varphi = \lim_{t \downarrow 0} A_t \varphi$. Our first goal is to show that $D(A)$ is dense. We use an idea similar to the technique used in the proof of Stone's theorem. For $\varphi \in X$, we set

$$\varphi_s = \int_0^s T(t)\varphi \, dt$$

Since $T(t)$ is strongly continuous, we need only use the Riemann integral.

For any $r > 0$, $T(r)\varphi_s = \int_0^s T(t + r)\varphi \, dt$; thus

$$\begin{aligned} A_r \varphi_s &= -\frac{1}{r} \int_0^s (T(t + r)\varphi - T(t)\varphi) \, dt \\ &= -\frac{1}{r} \int_s^{r+s} T(t)\varphi \, dt + \frac{1}{r} \int_0^r T(t)\varphi \, dt \\ &\xrightarrow[r \downarrow 0]{} -T(s)\varphi + \varphi \end{aligned}$$

Therefore, for each $\varphi \in X$ and $s > 0$, $\varphi_s \in D(A)$. Since $s^{-1}\varphi_s \to \varphi$ as $s \to 0$, A is densely defined. Furthermore, if $\varphi \in D(A)$, then $A_r T(t)\varphi = T(t)A_r \varphi$, so $T(t)$: $D(A) \to D(A)$ and

$$\frac{d}{dt} T(t)\varphi = -AT(t)\varphi = -T(t)A\varphi \tag{X.97}$$

A is also closed, for if $\varphi_n \in D(A)$, $\varphi_n \to \varphi$, and $A\varphi_n \to \psi$, then

$$\begin{aligned} \lim_{r \to 0} A_r \varphi &= \lim_{r \to 0} \lim_{n \to \infty} -\frac{1}{r} (T(r)\varphi_n - \varphi_n) \\ &= \lim_{r \to 0} \lim_{n \to \infty} \frac{1}{r} \int_0^r T(t) A\varphi_n \, dt \qquad \text{(by (X.97))} \\ &= \lim_{r \to 0} \frac{1}{r} \int_0^r T(t)\psi \, dt \\ &= \psi \end{aligned}$$

so $\varphi \in D(A)$ and $A\varphi = \psi$. We have thus proven:

Proposition Let $T(t)$ be a strongly continuous semigroup on a Banach space X and set $A\varphi = \lim_{r \to 0} A_r \varphi$ where $D(A) = \{\varphi \mid \lim_{r \downarrow 0} A_r \varphi \text{ exists}\}$. Then A is closed and densely defined. A is called the **infinitesimal generator** of $T(t)$. We will also say that A generates $T(t)$ and write $T(t) \equiv e^{-tA}$.

It is natural to ask what additional properties the generator of a contraction semigroup possesses. The formal Laplace transform

$$\frac{1}{\lambda + A} = -\int_0^\infty e^{-\lambda t} e^{-tA} \, dt$$

suggests that all μ with $\operatorname{Re} \mu < 0$ are in $\rho(A)$. This is in fact true and the formula holds in the strong sense. For suppose that $\operatorname{Re} \lambda > 0$. Then, since $\|e^{-tA}\| \leq 1$,

$$R\varphi = \int_0^\infty e^{-\lambda t}(e^{-tA}\varphi) \, dt$$

defines a bounded linear operator of norm less than or equal to $(\operatorname{Re} \lambda)^{-1}$. Moreover, for $r > 0$,

$$\begin{aligned} A_r R\varphi &= -\frac{1}{r} \int_0^\infty e^{-\lambda t}(e^{-(t+r)A} - e^{-tA})\varphi \, dt \\ &= \left(\frac{1 - e^{\lambda r}}{r} \right) \int_0^\infty e^{-\lambda t} e^{-tA}\varphi \, dt + \frac{e^{r\lambda}}{r} \int_0^r e^{-\lambda t} e^{-tA}\varphi \, dt \end{aligned}$$

so as $r \to 0$, $A_r R\varphi \to \varphi - \lambda R\varphi$. Thus $R\varphi \in D(A)$ and $AR\varphi = \varphi - \lambda R\varphi$ which implies $(\lambda + A)R\varphi = \varphi$. In addition, for $\varphi \in D(A)$ we have $AR\varphi = RA\varphi$ since

$$A \int_0^\infty e^{-\lambda t} e^{-tA}\varphi \, dt = \int_0^\infty e^{-\lambda t} A e^{-tA}\varphi \, dt = \int_0^\infty e^{-\lambda t} e^{-tA} A\varphi \, dt$$

The first equality follows by approximation with Riemann sums from the facts that $e^{-\lambda t}e^{-tA}\varphi$ and $Ae^{-\lambda t}e^{-tA}\varphi$ are integrable, A is closed. Thus, for $\varphi \in D(A)$, $R(\lambda + A)\varphi = \varphi = (\lambda + A)R\varphi$ which implies that

$$R = (\lambda + A)^{-1}$$

The properties of A which we have derived are also sufficient to guarantee that A generates a contraction semigroup. In fact, we only need information about real positive λ. This theorem (which we generalize later) is the analogue of Stone's theorem for self-adjoint operators.

Theorem X.47a (Hille–Yosida) A necessary and sufficient condition that a closed linear operator A on a Banach space X generate a contraction semigroup is that

(i) $(-\infty, 0) \subset \rho(A)$
(ii) $\|(\lambda + A)^{-1}\| \leq \lambda^{-1}$ for all $\lambda > 0$.

Furthermore, if A satisfies (i) and (ii), then the entire open left half-plane is contained in $\rho(A)$ and

$$(\lambda + A)^{-1}\varphi = -\int_0^\infty e^{-\lambda t} e^{-tA}\varphi \, dt \tag{X.98}$$

for all $\varphi \in X$ and λ with $\operatorname{Re}\lambda > 0$. Finally, if $T_1(t)$ and $T_2(t)$ are contraction semigroups generated by A_1 and A_2 respectively, then $T_2(t) \neq T_1(t)$ for some t implies that $A_1 \neq A_2$.

Proof Since we showed above that conditions (i) and (ii) are necessary and that (X.98) holds, we need only show sufficiency. So, suppose that A is a closed operator on X satisfying (i) and (ii). For $\lambda > 0$, define $A^{(\lambda)} = \lambda - \lambda^2(\lambda + A)^{-1}$. We will show that as $\lambda \to \infty$, $A^{(\lambda)} \to A$ strongly on $D(A)$ and then construct e^{-At} as the strong limit of the semigroups $e^{-tA^{(\lambda)}}$.

For $\varphi \in D(A)$, $A^{(\lambda)}\varphi = \lambda(\lambda + A)^{-1}A\varphi$. Moreover, by (ii),

$$\lambda(\lambda + A)^{-1}\varphi - \varphi = -(\lambda + A)^{-1}A\varphi \xrightarrow[\lambda \to \infty]{} 0$$

By condition (ii) the family $\{\lambda(\lambda + A)^{-1} \mid \lambda > 0\}$ is uniformly bounded in norm, so since $D(A)$ is dense, $\lambda(\lambda + A)^{-1}\psi \to \psi$ for all $\psi \in X$. Thus $A^{(\lambda)}\varphi \to A\varphi$ for all $\varphi \in D(A)$.

Since $A^{(\lambda)}$ is bounded, the semigroups $e^{-tA^{(\lambda)}}$ can be defined by power series. Since

$$\begin{aligned}\|e^{-tA^{(\lambda)}}\| &= \|e^{-\lambda t} e^{+t\lambda^2(\lambda+A)^{-1}}\| \\ &\leq e^{-\lambda t} \sum \frac{t^n \lambda^{2n}}{n!} \|(\lambda + A)^{-1}\|^n \\ &\leq 1\end{aligned}$$

they are contraction semigroups. For all μ, λ, $t > 0$, and all $\varphi \in D(A)$, we have

$$e^{-tA^{(\lambda)}}\varphi - e^{-tA^{(\mu)}}\varphi = \int_0^t \frac{d}{ds}\left(e^{-sA^{(\lambda)}} e^{-(t-s)A^{(\mu)}}\varphi\right) ds$$

so,

$$\begin{aligned}\|e^{-tA^{(\lambda)}}\varphi - e^{-tA^{(\mu)}}\varphi\| &\leq \int_0^t \|e^{-sA^{(\lambda)}} e^{-(t-s)A^{(\mu)}}\| \, \|A^{(\mu)}\varphi - A^{(\lambda)}\varphi\| \, ds \\ &\leq t\|A^{(\mu)}\varphi - A^{(\lambda)}\varphi\|\end{aligned}$$

We have used the fact that $e^{-(t-s)A^{(\mu)}}$ and $e^{-tA^{(\lambda)}}$ commute since $\{A^{(\lambda)}\}_{\lambda > 0}$ is a commuting family. Since we have proven above that $A^{(\lambda)}\varphi \to A\varphi$, $\{e^{-tA^{(\lambda)}}\varphi\}$ is Cauchy as $\lambda \to \infty$ for each $t > 0$ and $\varphi \in D(A)$. Since $D(A)$ is dense and the $e^{-tA^{(\lambda)}}$ are uniformly bounded, the same statement holds for all $\varphi \in X$. Now, define $T(t)\varphi = \lim_{\lambda \to \infty} e^{-tA^{(\lambda)}}\varphi$. $T(t)$ is a semigroup of contraction operators since these properties are preserved under strong limits. The above inequality shows that the convergence $e^{-tA^{(\lambda)}}\varphi \to T(t)\varphi$ is uniform for t restricted to a finite interval, so $T(t)$ is strongly continuous since $e^{-tA^{(\lambda)}}$ is. Thus, $T(t)$ is a contraction semigroup.

It remains to show that the infinitesimal generator of $T(t)$, call it $\tilde{A}$, is equal to A. For all t and $\varphi \in D(A)$,

$$e^{-tA^{(\lambda)}}\varphi - \varphi = -\int_0^t e^{-sA^{(\lambda)}} A^{(\lambda)}\varphi \, ds$$

so, since $A^{(\lambda)}\varphi \to A\varphi$, we have

$$T(t)\varphi - \varphi = -\int_0^t T(s)A\varphi \, ds$$

Thus, $\tilde{A}_t\varphi \to A\varphi$ as $t \to 0$. Therefore $D(\tilde{A}) \supset D(A)$ and $\tilde{A} \restriction D(A) = A$. For $\lambda > 0$, $(\lambda + A)^{-1}$ exists by hypothesis and $(\lambda + \tilde{A})^{-1}$ exists by the necessity part of the theorem. Thus $(\lambda + \tilde{A})D(\tilde{A}) = X = (\lambda + A)D(A)$, which implies that $D(\tilde{A}) = D(A)$.

Finally, suppose that $T_1(t)$ and $T_2(t)$ are contraction semigroups so that $T_1(t_0) \neq T_2(t_0)$ for some $t_0 > 0$. Then there is an $\ell \in X^*$ and a $\varphi \in X$ so that $\ell(T_1(t_0)\varphi) \neq \ell(T_2(t_0)\varphi)$. Since (X.98) holds for both $T_1(t)$ and $T_2(t)$, we conclude that $\ell((\lambda + A_1)^{-1}\varphi) \neq \ell((\lambda + A_2)^{-1}\varphi)$ for some λ with $\operatorname{Re}\lambda > 0$ because the ordinary Laplace transform is injective on the bounded functions. Thus, the resolvents of A_1 and A_2 differ, so $A_1 \neq A_2$. ∎

It is possible to construct e^{-tA} in the sufficiency part of Theorem X.47a by using the formula $e^{-tA} = \lim_{n \to \infty} (1 + (t/n)A)^{-n}$ (see Problem 49).

The difficulty in applying Theorem X.47a directly is that it is necessary to construct the resolvent of the closed operator A in order to verify conditions (i) and (ii). It is therefore convenient to have conditions on the operator A itself, that is, we seek an analogue of the symmetry condition and the fundamental criterion condition for self-adjoint operators. To see what these conditions should be, consider the Hilbert space case. If $\varphi \in D(A)$, then the fact that $\|e^{-tA}\varphi\|^2 \leq \|\varphi\|^2$ for all $t > 0$ implies that $(d/dt)\|e^{-tA}\varphi\|^2\big|_{t=0} \leq 0$. On the other hand,

$$\frac{d}{dt}\|e^{-tA}\varphi\|^2\Big|_{t=0} = -(A\varphi, \varphi) - (\varphi, A\varphi)$$

so we conclude that $\mathrm{Re}\,(A\varphi, \varphi) \geq 0$. Thus, we need to generalize the condition $\mathrm{Re}\,(A\varphi, \varphi) \geq 0$ to the Banach space case.

Definition Let X be a Banach space, $\varphi \in X$. An element $\ell \in X^*$ that satisfies $\|\ell\| = \|\varphi\|$, and $\ell(\varphi) = \|\varphi\|^2$ is called a **normalized tangent functional** to φ. By the Hahn–Banach theorem, each $\varphi \in X$ has at least one normalized tangent functional.

Definition A densely defined operator A on a Banach space X is called **accretive** if for each $\varphi \in D(A)$, $\mathrm{Re}(\ell(A\varphi)) \geq 0$ for some normalized tangent functional to φ. A is called **maximal accretive** (or **m-accretive**) if A is accretive and A has no proper accretive extension.

We remark that an accretive operator is closable (Problem 52). The closure of an accretive operator is again accretive, so every accretive operator has a smallest closed accretive extension. We can now state the fundamental criterion.

Theorem X.48 A closed operator A on a Banach space X is the generator of a contraction semigroup if and only if A is accretive and $\mathrm{Ran}(\lambda_0 + A) = X$ for some $\lambda_0 > 0$.

Proof Let e^{-tA} be a contraction semigroup and suppose that ℓ is any normalized tangent functional to $\varphi \in D(A)$. Then $\ell(e^{-tA}\varphi)$ is differentiable and

$$\frac{d}{dt}\,\mathrm{Re}(\ell(e^{-tA}\varphi))\bigg|_{t=0} = -\mathrm{Re}\,\ell(A\varphi)$$

On the other hand

$$|\ell(e^{-tA}\varphi)| \leq \|\ell\|\,\|e^{-tA}\varphi\| \leq \|\varphi\|^2 = \ell(\varphi)$$

for all $t > 0$, so $\mathrm{Re}\,t^{-1}(\ell(e^{-tA}\varphi) - \ell(\varphi)) \leq 0$ for all $t > 0$. Thus,

$$-\mathrm{Re}(\ell(A\varphi)) \leq 0$$

for all normalized tangent functionals to φ, so A is accretive. The fact that $\mathrm{Ran}(I + A) = X$ is a consequence of (i) in Theorem X.47a. This proves necessity.

To show sufficiency, suppose $\lambda > 0$ and A is a closed accretive operator satisfying $\mathrm{Ran}(\lambda_0 + A) = X$, for some $\lambda_0 > 0$. Let ℓ be a normalized tangent

functional to $\varphi \in D(A)$ so that $\mathrm{Re}(\ell(A\varphi)) \geq 0$. Then

$$\begin{aligned}\lambda\|\varphi\|^2 &\leq \lambda\ell(\varphi) + \mathrm{Re}\,\ell(A\varphi)\\ &= \mathrm{Re}\,\ell((\lambda + A)\varphi)\\ &\leq \|\varphi\|\,\|(\lambda + A)\varphi\|\end{aligned}$$

Thus, $\mathrm{Ran}(\lambda + A)$ is closed and $\lambda + A$ has a bounded inverse from $\mathrm{Ran}(\lambda + A)$ to $D(A)$ of norm less than or equal to λ^{-1}. To complete the proof we need only show that $\mathrm{Ran}(\lambda + A)$ is dense. But $\mathrm{Ran}(\lambda + A)$ is dense for $\lambda = \lambda_0$, so the usual perturbation argument (see the proof of Theorem X.1) shows that $\mathrm{Ran}(\lambda + A)$ is dense for all $\lambda > 0$. ∎

Corollary Let A be a closed operator on a Banach space X. Then, if both A and its adjoint A' are accretive, A generates a contraction semigroup.

Proof Suppose that $\mathrm{Ran}(I + A)$ is not dense. Then by the Hahn–Banach theorem there is an $\ell \in X^*$ so that $\ell((I + A)\varphi) = 0$ for all $\varphi \in D(A)$. Thus, $\ell \in D(A')$ and $(I + A')\ell = 0$. So, if μ is any normalized tangent functional to ℓ in X^{**}, $\mu(A'\ell) = -\|\ell\|^2$, which contradicts the assumption that A' is accretive unless $\ell = 0$. Thus, $\mathrm{Ran}(I + A)$ is dense. ∎

Before giving some examples, we make several remarks. First, to prove sufficiency in Theorem X.48, we used only the assumption that there exists at least one normalized tangent functional ℓ for each $\varphi \in D(A)$ with $\mathrm{Re}\,\ell(A\varphi) \geq 0$. From this it followed that $(\lambda + A)^{-1}$ was bounded for each $\lambda > 0$. Using the further assumption that $\mathrm{Ran}(\lambda_0 + A) = X$ we then concluded the proof of sufficiency. However, the necessity part of the argument showed that if A generates a contraction semigroup, then $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for *all* tangent functionals. Thus, in the presence of the assumption $\mathrm{Ran}(I + A) = X$, the condition that $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for one tangent functional (for each $\varphi \in D(A)$) implies $\mathrm{Re}\,\ell(A\varphi) \geq 0$ for all tangent functionals. Secondly, the generators of contraction semigroups are clearly maximal accretive since the condition $\mathrm{Ran}(I + A) = X$ implies that A has no proper accretive extensions. The converse statement, i.e., if A is maximal accretive, then A generates a contraction semigroup, holds in the Hilbert space case but not in the Banach space case (see the Notes and Problem 50). Finally, as in the case of self-adjoint operators, there is a core theorem for the generators of contraction semigroups:

Theorem X.49 Let A be the generator of a contraction semigroup on a Banach space X. Let D be a dense set, $D \subset D(A)$, so that $e^{-tA}\colon D \to D$. Then D is a core for A (i.e., $\overline{A \restriction D} = A$).

Proof Let $\lambda > 0$. We need only show that $\mathrm{Ran}(\lambda + A \restriction D)$ is dense. Suppose not. Then there is a $\ell \in X^*$, $\ell \neq 0$, so that $\ell((\lambda + A)\varphi) = 0$ for all $\varphi \in D$. But, if $\varphi \in D$,

$$\frac{d}{dt}\ell(e^{-tA}\varphi) = \ell(-Ae^{-tA}\varphi) = \lambda\ell(e^{-tA}\varphi)$$

since $e^{-tA}\varphi \in D$. Thus $\ell(e^{-tA}\varphi) = \ell(\varphi)e^{\lambda t}$ which for large enough t contradicts the fact that e^{-tA} is a contraction unless $\ell(\varphi) = 0$. Since D is dense, $\ell(\varphi)$ cannot equal zero for all $\varphi \in D$, so we conclude that $\mathrm{Ran}(\lambda + A \restriction D)$ is dense. ∎

Example 1 Let B be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Then $\|(\mu - B)^{-1}\| \leq |\mathrm{Im}\,\mu|^{-1}$, so the operators $A_1 = iB$ and $A_2 = -iB$ both satisfy the hypotheses of the Hille–Yosida theorem. The contraction semigroups e^{-tA_1}, and e^{-tA_2} are equal to the unitary groups e^{itB} for $t < 0$ and $t > 0$ respectively.

If $B \geq 0$, then B itself satisfies the hypotheses of the Hille–Yosida theorem since $\|(\mu + B)^{-1}\| \leq \mu^{-1}$ for $\mu > 0$ by the functional calculus. Thus, B generates a contraction semigroup e^{-Bt}. Of course, these semigroups can be constructed directly from the functional calculus.

Example 2 (the heat equation on $L^2(\mathbb{R}^n)$) The operator $-\Delta$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R}^n)$ and positive so its closure (which we also denote by $-\Delta$) generates a semigroup $e^{\Delta t}$ on $L^2(\mathbb{R}^n)$. For $f \in L^2(\mathbb{R}^n)$, we define $u(x, t) = e^{\Delta t}f$. Then for all $\varphi \in C_0^\infty(\mathbb{R}^n \times (0, \infty))$,

$$\begin{aligned}
&\int_{\mathbb{R}^{n+1}} \overline{\left(\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} u(x, t)\, dx\, dt \\
&\quad = \int_{\mathbb{R}} \left(\int_{\mathbb{R}^n} \overline{\left(\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} e^{\Delta t} f(x)\, dx \right) dt \\
&\quad = \int_{\mathbb{R}} \left(\int_{\mathbb{R}^n} \overline{\left(e^{\Delta t}\left(-\frac{\partial}{\partial t} - \Delta\right)\varphi(x, t)\right)} f(x)\, dx \right) dt \\
&\quad = \int_{\mathbb{R}} \int_{\mathbb{R}^n} -\frac{\partial}{\partial t}[\overline{(e^{\Delta t}\varphi)(x, t)} f(x)]\, dx\, dt \\
&\quad = 0
\end{aligned}$$

so $u(x, t)$ is a weak solution of the heat equation $\partial u(x, t)/\partial t = \Delta u(x, t)$. If $f \in D(\Delta)$, then for each $t > 0$, $u(x, t) \in D(\Delta)$ as a function of x, so in this case $u(x, t)$ is a classical solution in the sense that $u(x, t)$ is an $L^2(\mathbb{R}^n)$-valued differentiable function of t and $\partial u(x, t)/\partial t = \Delta u(x, t)$. In either case $u(x, t)$ satisfies the initial condition $u(x, 0) = f(x)$ in the sense that $\|u(x, t) - f(x)\|_{L^2(\mathbb{R}^n)} \to 0$ as $t \to 0$. We will see later that for $t > 0$, $u(x, t)$ is in fact infinitely differentiable in x and t for all $f \in L^2(\mathbb{R}^n)$. We remark that since $e^{\Delta t}$ is a contraction semigroup $\|u(x, t)\|_{L^2(\mathbb{R}^n)}$ is a nonincreasing function of t.

Example 3 (the heat equation on $C_\infty(\mathbb{R}^n)$) We denote by $C_\infty(\mathbb{R}^n)$ the continuous functions on $\mathbb{R}^n$ with $f(x) \to 0$ as $|x| \to \infty$. $C_\infty(\mathbb{R}^n)$ is a Banach space under the sup norm. We define $-\Delta$ as the closure of the operator $\varphi \to -\Delta\varphi$ on $\mathscr{S}(\mathbb{R}^n)$. We will show that $-\Delta$ satisfies the hypotheses of Theorem X.48. Let $\varphi \in \mathscr{S}(\mathbb{R}^n)$. Then there is a point x_0 so that $|\varphi(x_0)| = \sup_{x \in \mathbb{R}^n} |\varphi(x)|$. Let $\ell_\varphi = \overline{\varphi(x_0)}\delta_{x_0}$. Then $\ell_\varphi \in C_\infty(\mathbb{R}^n)^*$, $\|\ell_\varphi\| = |\varphi(x_0)| = \|\varphi\|$, and $\ell(\varphi) = |\varphi(x_0)|^2 = \|\varphi\|^2$, so ℓ is a normalized tangent functional to φ. Further,

$$\begin{aligned}
\mathrm{Re}(\ell_\varphi(-\Delta\varphi)) &= \mathrm{Re}\ \overline{\varphi(x_0)}(-\Delta\varphi(x_0)) \\
&= |\nabla\varphi(x_0)|^2 - \tfrac{1}{2}\Delta|\varphi(x_0)|^2 \\
&\geq 0
\end{aligned}$$

because $\Delta|\varphi(x_0)|^2 \leq 0$ since $|\varphi(x)|^2$ has its maximum at x_0. This shows that $-\Delta \restriction \mathscr{S}(\mathbb{R}^n)$ is accretive, and thus its closure is accretive. Moreover, if $g \in \mathscr{S}(\mathbb{R}^n)$, $\widehat{(1 + k^2)^{-1}\hat{g}} \in \mathscr{S}(\mathbb{R}^n) \subset D(-\Delta)$ and $(I - \Delta)\widehat{(1 + k^2)^{-1}\hat{g}} = g$ so $\mathrm{Ran}(I - \Delta)$ contains $\mathscr{S}(\mathbb{R}^n)$ which is dense in $C_\infty(\mathbb{R}^n)$. Since $\mathrm{Ran}(I - \Delta)$ is closed, we conclude that $\mathrm{Ran}(I - \Delta) = C_\infty(\mathbb{R}^n)$. Thus, $-\Delta$ is accretive and satisfies $\mathrm{Ran}(I - \Delta) = C_\infty(\mathbb{R}^n)$, so by Theorem X.48, $-\Delta$ generates a contraction semigroup $e^{\Delta t}$ on $C_\infty(\mathbb{R}^n)$. As in Example 2, it may be shown that for $f \in C_\infty(\mathbb{R}^n)$, $u(x, t) = e^{\Delta t}f$ is a weak solution of the heat equation. We will see later that $u(x, t)$ is in fact a strict solution. $u(x, t)$ satisfies the initial condition $u(x, 0) = f(x)$ in the sense that

$$\sup_{x \in \mathbb{R}^n} |u(x, t) - f(x)| \to 0 \qquad \text{as} \quad t \to 0$$

Since $e^{\Delta t}$ is a contraction semigroup, $\max_{x \in \mathbb{R}^n} |u(x, t)|$ is a nonincreasing function of t. This reflects the intuitive notion that the maximum temperature should decrease as the heat diffuses.

Since $e^{t\Delta}$ has an explicit kernel, we could have analyzed Examples 2 and 3 by "direct" methods. The advantage of the abstract theory is in cases where there is no explicit solution available. See, for instance, Example 4, p. 245.

There is also a perturbation theorem for generators of contraction semigroups analogous to the Kato–Rellich theorem. We first prove a lemma which we later strengthen.

Lemma Let A be the generator of a contraction semigroup on a Banach space X. Suppose that B is an accretive operator, with $D(B) \supset D(A)$, and

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|$$

for some b, some $a < \frac{1}{2}$, and all $\varphi \in D(A)$. Then $A + B$ (defined on $D(A)$) is a closed accretive operator and generates a contraction semigroup.

Proof The idea of the proof is the same as the proof of Theorem X.12. Let $\lambda > 0$. Then $\|A(\lambda + A)^{-1}\| = \|\lambda(\lambda + A)^{-1} - 1\| \leq 2$. Thus for $\varphi \in D(A)$,

$$\|B(\lambda + A)^{-1}\varphi\| \leq a\|A(\lambda + A)^{-1}\varphi\| + b\|(\lambda + A)^{-1}\varphi\|$$

$$\leq \left(2a + \frac{b}{\lambda}\right)\|\varphi\|$$

Thus, for λ sufficiently large, $\|B(\lambda + A)^{-1}\| < 1$. Therefore, since

$$\mathrm{Ran}(\lambda + \mathrm{A}) = X$$

and

$$(\lambda + A + B) = (I + B(\lambda + A)^{-1})(\lambda + A)$$

we conclude that $\mathrm{Ran}(\lambda + A + B) = X$. Since A generates a contraction semigroup, we know that $\mathrm{Re}(\ell(A\varphi)) \geq 0$ for *every* normalized tangent functional to φ. Thus $A + B$ is accretive and generates a contraction semigroup. ∎

Theorem X.50 Let A and C be accretive operators on a Banach space X. Suppose that there is a dense set D, $D \subset D(A)$, $D \subset D(C)$, and an $a \in [0, 1)$ so that

$$\|(A - C)\varphi\| \leq a(\|A\varphi\| + \|C\varphi\|) + b\|\varphi\|$$

for some b and all $\varphi \in D$. Then

(a) $\bar{A}$ generates a contraction semigroup if and only if $\bar{C}$ does.
(b) $D(\overline{A \restriction D}) = D(\overline{C \restriction D})$.

Proof To prove (a), one need only show that $\mathrm{Ran}(\lambda_0 + A)$ is dense for some $\lambda_0 > 0$ if and only if $\mathrm{Ran}(\mu_0 + C)$ is dense for some $\mu_0 > 0$. The proof is exactly the same as the proof of Theorem X.13 except that we choose α' so that $2a\alpha'/(1 - a) < \frac{1}{2}$ so we can use the lemma. As before, part (b) is left to the reader. ∎

Corollary Let A and B satisfy all the hypotheses of the lemma except that the condition $a < \frac{1}{2}$ is replaced by $a < 1$. Then the conclusion of the lemma holds.

As in the case of self-adjoint operators we have a product formula:

Theorem X.51 (the Trotter product formula) Let A and B be the generators of contraction semigroups on a Banach space X. Suppose that the closure of $(A + B) \restriction D(A) \cap D(B)$ generates a contraction semigroup on X. Then, for all $\varphi \in X$,

$$e^{-t(\overline{A+B})}\varphi = \lim_{n\to\infty} (e^{-tA/n}e^{-tB/n})^n\varphi$$

In the case where $D = D(A) \cap D(B)$ and $(A + B) \restriction D$ is closed, the proof of Theorem X.41 is exactly the same as the proof given in Theorem VIII.30. For the general case, see the references in the Notes.

Example 4 (the heat equation with sources and sinks proportional to the temperature) Let $q(x)$ be a bounded ($|q(x)| < M$), real-valued continuous function on $\mathbb{R}^n$. The differential equation

$$\frac{\partial}{\partial t}u(x, t) - \Delta u(x, t) = -q(x)u(x, t) \tag{X.99}$$

corresponds to the physical situation where a source adds (if $q(x) \leq 0$) or subtracts (if $q(x) \geq 0$) heat at the point x proportionally to the local temperature at x at time t. Our previous discussion suggests that we consider the operator

$$A = -\Delta + q(x)$$

on $L^2(\mathbb{R}^n)$ and $C_\infty(\mathbb{R}^n)$. Since $q(x)$ is bounded by M as an operator on $L^2(\mathbb{R}^n)$, the Kato–Rellich theorem immediately implies that A is self-adjoint on $D(-\Delta)$ and bounded below by $-M$. Thus, e^{-tA} can be defined by using the functional calculus and if $f \in D(-\Delta)$, then $u(x, t) = e^{-At}f$ satisfies (X.99) with initial conditions $u(x, 0) = f(x)$.

In the case of $C_\infty(\mathbb{R}^n)$ we use the corollary to Theorem X.50, the Banach space analogue of the Kato–Rellich theorem. Suppose first that $q(x) \geq 0$. Then multiplication by $q(x)$ is a bounded accretive operator on $D(-\Delta) \subset C_\infty(\mathbb{R}^n)$ for we can use the same normalized tangent functionals, ℓ_φ as in Example 3, and find that $\ell_\varphi(q\varphi) = q(x_0)|\varphi(x_0)|^2 \geq 0$. Thus, by the corollary to Theorem X.50, A is a closed accretive operator on $D(-\Delta)$.

As before, $u(x, t) = e^{-At}f$ satisfies (X.99) weakly and $\|u(x, t) - f(x)\|_\infty \to 0$ as $t \to \infty$.

If q is negative at any point, then multiplication by q is *not* accretive on $C_\infty(\mathbb{R}^n)$. This is natural since we would only expect e^{-tA} to be a contraction semigroup if $q(x) \geq 0$ (i.e., if heat is only absorbed but not added). But, we can easily surmount this difficulty by defining $A_M = -\Delta + q(x) + M$ on $D(-\Delta)$. Since $q(x) + M \geq 0$, $q(x) + M$ is a bounded accretive operator, and we can apply the corollary to construct the contraction semigroup e^{-tA_M}. We now set $T(t) = e^{tM}e^{-tA_M}$. Then $T(t)$ is a strongly continuous semigroup and for each $f \in D(-\Delta)$, $u(x, t) = T(t)f$ satisfies (X.99) weakly.

Intuitively, the solution of the heat equation should be positivity preserving, i.e., if $u(x, 0) \geq 0$ a.e., then $u(x, t) \geq 0$ a.e. $[x]$ for each $t > 0$. In Problem 53, the reader is asked to show that $e^{\Delta t}$ is positivity preserving on $L^2(\mathbb{R}^n)$. Since $e^{-tq(x)} \geq 0$ for all x, $(e^{\Delta t/n}e^{-tq(x)/n})^n f \geq 0$ if $f \geq 0$. By the Trotter product formula

$$(e^{\Delta t/n}e^{-tq(x)/n})^n f \xrightarrow[n\to\infty]{L^2} e^{-t(-\Delta+q)}f$$

so we must have $e^{-t(-\Delta+q)}f \geq 0$ a.e. A similar use of Trotter's formula shows that $T(t) = e^{tM}e^{-t(-\Delta+q+M)}$ is positivity preserving on $C_\infty(\mathbb{R}^n)$ (Problem 54).

The construction of $e^{-(-\Delta+q)t}$ in Example 4, in the case where $q \leq 0$, shows that strongly continuous semigroups which are not contraction semigroups arise naturally. So we will now show how the results for contraction semigroups can be easily generalized. Let $T(t)$ be a strongly continuous semigroup and let $\alpha > 0$. Since $t \mapsto T(t)\varphi$ is continuous and $[0, \alpha]$ is compact, the set $\{\|T(t)\varphi\|, 0 \leq t \leq \alpha\}$ is bounded. Thus, the uniform boundedness principle (Theorem III.9) implies that there is an M so that $\|T(t)\| \leq M$ for all $t \in [0, \alpha]$. Now let $t \in (0, \infty)$. Then we can write $t = n\alpha + \tau$, where $\tau \in [0, \alpha]$. Thus, by the semigroup property

$$\|T(t)\| = \|T(\alpha)^n T(\tau)\| \leq M^{n+1} \leq Me^{\omega t}$$

where $\omega = \alpha^{-1} \log M$. Therefore, all strongly continuous semigroups are exponentially bounded. The inf of the numbers ω so that there is an M with $\|T(t)\| \leq Me^{\omega t}$ is denoted by ω_0 and called the **type** of the semigroup (see Problem 51). We define the **generator** A of $T(t)$ in exactly the same way as for contraction semigroups. As before A is closed and an

argument almost identical to that given before Theorem X.47a shows that if $\lambda > \omega_0$, then $-\lambda \in \rho(A)$ and

$$(\lambda + A)^{-1}\varphi = \int_0^\infty e^{-\lambda t}T(t)\varphi \, dt$$

for all $\varphi \in X$. Thus, if $\omega > \omega_0$ and $\lambda > \omega$,

$$\begin{aligned}\|(\lambda + A)^{-n}\varphi\| &= \left\| \frac{(-1)^n}{n!}\left(\frac{d}{d\lambda}\right)^n (\lambda + A)^{-1}\varphi \right\| \\ &\leq \frac{1}{n!}\left(\int_0^\infty t^n e^{-\lambda t} M e^{\omega t}\, dt\right)\|\varphi\| \\ &= \frac{M\|\varphi\|}{(\lambda - \omega)^n}\end{aligned}$$

Conversely, a few minor changes in the proof of Theorem X.47a show that these conditions are also sufficient for A to generate a strongly continuous semigroup (Problem 55). Thus, we have:

Theorem X.47b (the Hille–Yosida–Phillips theorem) A necessary and sufficient condition for a closed operator A on a Banach space X to generate a strongly continuous semigroup is that

(i) There is an $\omega > 0$ so that each $\lambda > \omega$ is in $\rho(A)$.
(ii) There is an M so that

$$\|(\lambda + A)^{-n}\| \leq \frac{M}{(\lambda - \omega)^n}$$

for all $\lambda > \omega$ and all positive integers n.

In this case we have $\|e^{-tA}\| \leq Me^{\omega t}$ for all $t > 0$ and

$$\|(\lambda + A)^{-1}\| \leq \frac{M}{\mathrm{Re}(\lambda - \omega)}$$

for all λ so that $\mathrm{Re}(\lambda - \omega) > 0$.

Our last topic in this section is the theory of bounded holomorphic semigroups. To see what we are after, consider first the case of a positive self-adjoint operator A in a Hilbert space $\mathscr{H}$. The vector-valued function $e^{-tA}\varphi$ can be analytically continued to the right-half plane by using the functional calculus. This suggests:

Definition Let $\theta \in (0, \pi/2]$. A strongly continuous bounded semigroup $T(t)$, $t > 0$ on a Banach space X is called a **bounded holomorphic semigroup of angle** θ if:

(i) $T(t)$ is the restriction to the positive real axis of an analytic family of operators $T(z)$ in the open sector $S_\theta = \{z \mid |\arg z| < \theta\}$ which obeys $T(z + z') = T(z)T(z')$ for all $z, z' \in S_\theta$.

(ii) For each $\theta_1 < \theta$, $T(z)$ is uniformly bounded in the sector S_{θ_1} and $T(z)\varphi \to \varphi$ if $z \to 0$ in S_{θ_1} for all $\varphi \in X$.

If A is the infinitesimal generator of $T(t)$, we write $T(z) = e^{-zA}$.

We can easily derive several properties of the generator A of a bounded holomorphic semigroup of angle θ. For each $0 < \eta < \theta$, $e^{-(re^{i\eta})A}$ is a bounded strongly continuous semigroup (as a function of r). It is clear that its generator is $e^{i\eta}A$, so the spectrum of $e^{i\eta}A$ must be contained in the right half-plane. Since this is true for all η satisfying $0 \leq |\eta| < \theta$, we conclude that

$$\sigma(A) \subset \overline{S}_{\pi/2-\theta} \equiv \left\{ z \,\middle|\, |\arg z| \leq \frac{\pi}{2} - \theta \right\} \tag{X.100}$$

Furthermore, for each $\theta_1 < \theta$, $e^{-(re^{i\eta})A}$ is uniformly bounded (say by M_1) for all $r > 0$ and all η with $|\eta| \leq \theta_1$. Thus, by Theorem X.47b,

$$\|(\lambda + e^{i\eta}A)^{-1}\| \leq \frac{M_1}{\operatorname{Re}(\lambda)}$$

for all λ with $\operatorname{Re} \lambda > 0$. It follows that, given $\theta_1 < \theta$,

$$\|(z + A)^{-1}\| \leq \frac{M_1}{\operatorname{dist}(z, \overline{S}_{\pi/2-\theta_1})} \tag{X.101}$$

for all $z \in \mathbb{C} \backslash \overline{S}_{\pi/2-\theta_1}$ where M_1 depends on θ_1.

In fact, these conditions are also sufficient:

Theorem X.52 A closed operator A on a Banach space X is the generator of a bounded holomorphic semigroup of angle $\theta \leq \pi/2$ if and only if A satisfies conditions (X.100) and (X.101).

Proof We have already proven necessity. We remark that we could prove sufficiency by the same method as in the Hille–Yosida theorem if we had the stronger hypothesis

$$\|(z + A)^{-n}\| \leq \frac{M_1}{(\operatorname{dist}(z, \overline{S}_{\pi/2-\theta_1}))^n}, \qquad n = 1, 2, \ldots \tag{X.101a}$$

instead of (X.101). In most applications, one can verify (X.101a), but the proof of the general case is instructive. The idea of the proof is to use a generalization of the Dunford functional calculus (see Problem 1 and the notes in Chapter VII) to define a semigroup which we then show has the right properties. Let $0 < \theta_2 < \theta_1 < \theta$ and let Γ be the path indicated in Figure X.5. We define

$$T(z) \equiv -\frac{1}{2\pi i} \int_\Gamma e^{-\lambda z} (\lambda - A)^{-1} \, d\lambda \tag{X.102}$$

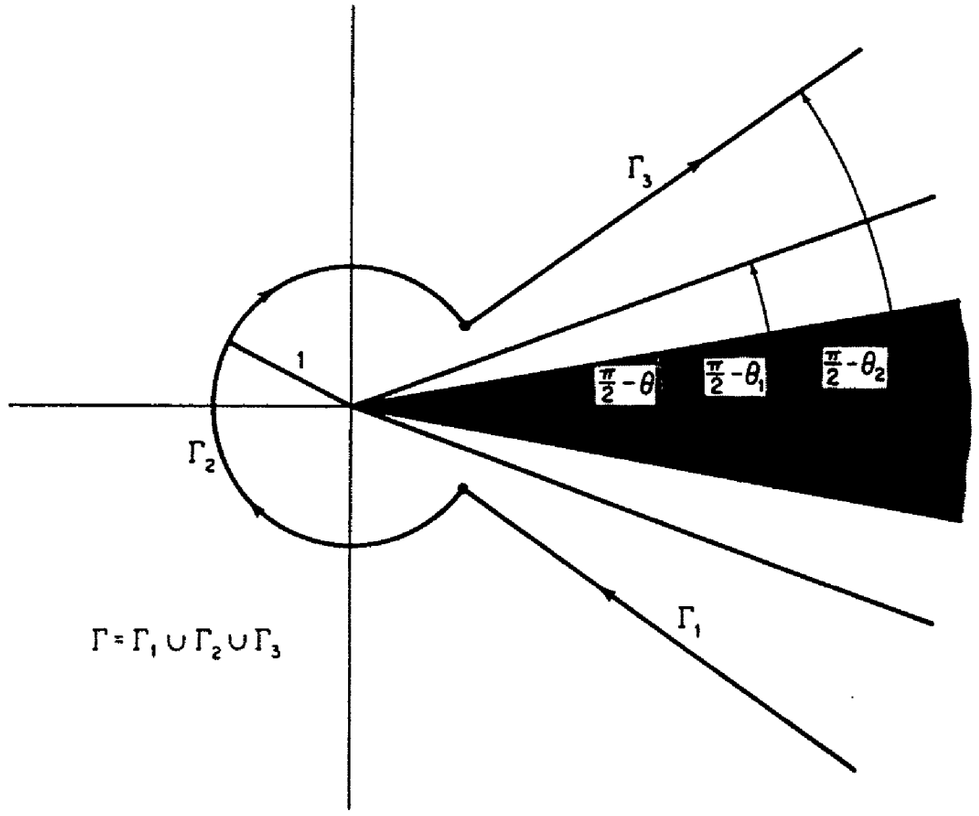


FIGURE X.5 The curve Γ.

for all $z \in S_{\theta_2} = \{z \mid |\arg z| < \theta_2\}$. Since $\sigma(A) \subset \overline{S}_{\pi/2-\theta}$, $(\lambda - A)^{-1}$ is well defined on Γ. Moreover, for $\lambda \in \Gamma_1 \cup \Gamma_3$, $\operatorname{Re}(z\lambda) = c(z)|\lambda|$ where $c(z) = |z|\cos(\arg z + \pi/2 - \theta_2)$, so for $z \in S_{\theta_2}$ the integral converges and $\|T(z)\|$ is uniformly bounded in the region

$$R_{\varepsilon,\delta} = \{z \mid |z| \geq \delta, |\arg z| \leq \theta_2 - \varepsilon\}$$

for each $\varepsilon, \delta > 0$. On the other hand if $0 < |z| \leq \delta$ and $|\arg z| \leq \theta_2 - \varepsilon$, then making the change of variables $\zeta = |z|\lambda$, we find

$$T(z) = \int_{\Gamma'} e^{-\zeta z/|z|}\left(\frac{\zeta}{|z|} - A\right)^{-1} \frac{d\zeta}{|z|}$$

(see Figure X.6)

$$= \int_{\Gamma} e^{-\zeta z/|z|}\left(\frac{\zeta}{|z|} - A\right)^{-1} \frac{d\zeta}{|z|}$$

(by the Cauchy integral formula and (X.101)).

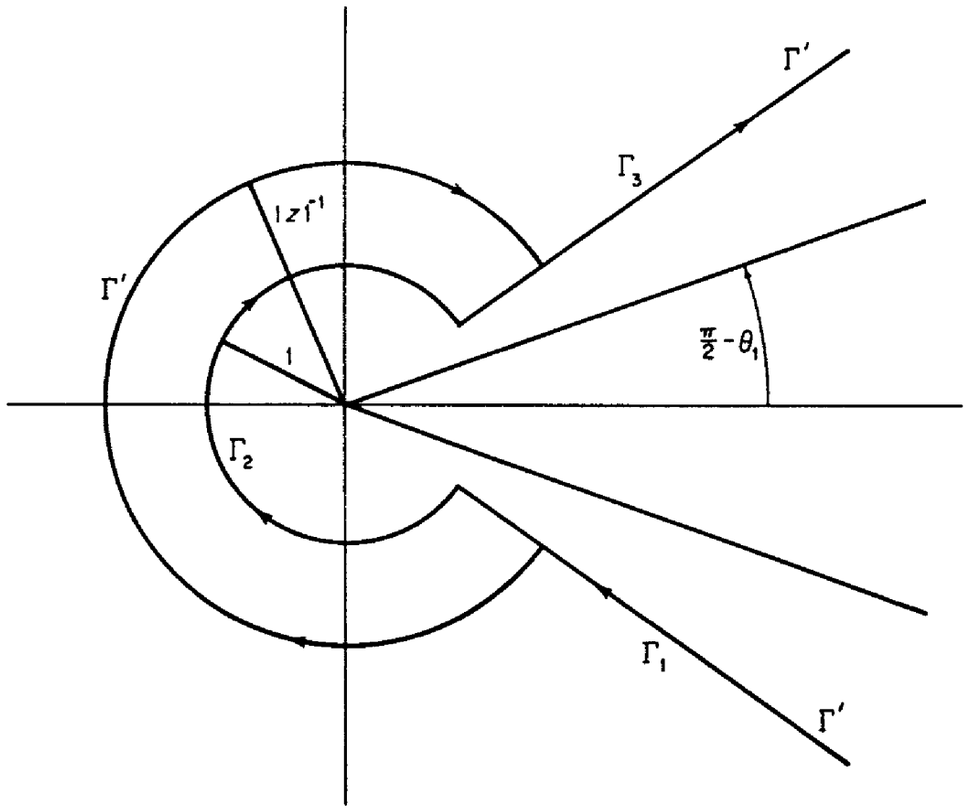


FIGURE X.6 The curve Γ'.

Since for $\zeta \in \Gamma$, $\operatorname{dist}(\zeta/|z|, \bar{S}_{\pi/2-\theta_1}) = |z|^{-1} \operatorname{dist}(\zeta, \bar{S}_{\pi/2-\theta_1})$,

$$\|e^{-zA}\| \leq \int_{\Gamma_1 \cup \Gamma_3} e^{-|\zeta|(1-\cos(\pi/2-\varepsilon))} M_1 \, d\zeta + C$$

$$\leq C_1 \qquad \text{(independently of } z\text{)}$$

so $T(z)$ is uniformly bounded in the sector $R_{\varepsilon,0} = \bar{S}_{\theta_2-\varepsilon}$. Furthermore, $T(z)$ is an analytic operator-valued function in S_{θ_2} since we may differentiate under the integral sign.

To prove that $T(z)$ is a semigroup, we proceed as follows. Let Γ'' be the curve Γ shifted to the left by two units. Then by Cauchy's theorem and (X.101), the definition of $T(z)$ is independent of whether we use Γ or Γ'' to define $T(z)$. Let $z, z' \in S_{\theta_2}$. Then, using Fubini's theorem, the first resolvent formula, and the Cauchy integral formula, we find

$$T(z)T(z') = \left(\frac{1}{2\pi i}\right)^2 \int_{\Gamma}\int_{\Gamma''} e^{-\lambda z - \mu z'}(\lambda - A)^{-1}(\mu - A)^{-1} \, d\mu \, d\lambda$$

$$= \left(\frac{1}{2\pi i}\right)^2 \int_{\Gamma}\int_{\Gamma''} e^{-\lambda z - \mu z'}(\mu - \lambda)^{-1}((\lambda - A)^{-1} - (\mu - A)^{-1}) \, d\mu \, d\lambda$$

$$= -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda(z+z')}(\lambda - A)^{-1} \, d\lambda$$

$$= T(z + z').$$

Now, suppose that $z \to 0$ in the sector $\bar{S}_{\theta_2-\varepsilon}$ and $\varphi \in D(A)$. Then

$$T(z)\varphi - \varphi = -\frac{1}{2\pi i}\int_{\Gamma} (e^{-\lambda z}(\lambda - A)^{-1} - e^{-\lambda z}\lambda^{-1})\varphi \, d\lambda$$

$$= -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}\lambda^{-1}(\lambda - A)^{-1}A\varphi \, d\lambda$$

$$\xrightarrow[z\to 0]{} -\frac{1}{2\pi i}\int_{\Gamma} \lambda^{-1}(\lambda - A)^{-1}A\varphi \, d\lambda \qquad \text{(by the dominated convergence Theorem and (X.101))}$$

$$= 0 \qquad \text{(by Cauchy's theorem, (X.100), and (X.101))}$$

Since the $T(z)$ are uniformly bounded. $T(z)\varphi \to \varphi$ for all $\varphi \in X$. Thus, $T(z)$ is a strongly continuous semigroup in $\bar{S}_{\theta_2-\varepsilon}$, in particular $T(t)$ is strongly continuous for $t > 0$.

Let $\varphi \in X$. Then as remarked above, we may differentiate under the integral sign to obtain

$$\frac{d}{dz}T(z)\varphi = -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}(-\lambda)(\lambda - A)^{-1}\varphi \, d\lambda$$

$$= -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}(-\varphi - A(\lambda - A)^{-1}\varphi) \, d\lambda$$

$$= -\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}(-A(\lambda - A)^{-1}\varphi) \, d\lambda \qquad \text{(Cauchy's theorem)}$$

$$= -A\left[-\frac{1}{2\pi i}\int_{\Gamma} e^{-\lambda z}(\lambda - A)^{-1}\varphi \, d\lambda\right] \qquad \text{(since } A \text{ is closed)}$$

$$= -AT(z)\varphi$$

Thus, $T(z)$: $X \to D(A)$ and $-AT(z)\varphi = T'(z)\varphi$. Further, if $\varphi \in D(A)$, the same calculation shows that $T'(z)\varphi = -T(z)A\varphi$. Thus, the vector-valued function $T(t)\varphi$ has a uniformly bounded derivative for $t > 0$ so

$$\frac{T(t)\varphi - \varphi}{t} = \frac{1}{t}\int_0^t T'(s)\varphi \, ds$$

$$= \frac{1}{t}\int_0^t -AT(s)\varphi \, ds$$

$$\xrightarrow[t\to 0]{} -A\varphi$$

Thus, the generator of $T(t)$ extends A, but since $T(t)$: $D(A) \to D(A)$, Theorem X.49 implies that A itself generates $T(t)$.

Since θ_2 may be taken as close to θ_1 as we like and $\varepsilon > 0$ was arbitrary, we have proven the theorem. ∎

Corollary 1 Let q be a strictly m-accretive form on a Hilbert space $\mathscr{H}$ so that $\varphi \in Q(q)$ implies $|\arg[q(\varphi, \varphi)]| \leq \theta$ where $\theta < \pi/2$. Then the associated strictly m-accretive operator (given in Theorem VIII.16) generates a bounded holomorphic semigroup of angle $\pi/2 - \theta$.

Proof The corollary follows immediately from Theorem VIII.17 and the theorem above. ∎

Corollary 2 Let A be the generator of a bounded holomorphic semigroup of angle θ, $\theta > 0$. Then for each integer $m > 0$ and each $\varphi \in X$, $e^{-tA}\varphi \in D(A^m)$ and $\|A^m e^{-tA}\varphi\| \leq C\|\varphi\|/|t|^m$ for all $t > 0$ (C depends on A and m but not on φ).

The proof of this corollary just uses the representation (X.102), the formula $T'(z) = -AT(z)$, and manipulations similar to those in the theorem. The details are left as Problem 58.

The notion of bounded holomorphic semigroup can be generalized in the same way that we generalized the notion of contraction semigroup. A strongly continuous semigroup $T(t)$ on a Banach space X is called a **holomorphic semigroup of angle** θ if $T(t)$ satisfies all the properties of a bounded holomorphic semigroup of angle θ except that it is not required to be uniformly bounded in sectors $\bar{S}_{\theta_1}$, $\theta_1 < \theta$. If $T(t)$ is a holomorphic semigroup of angle θ, then for each $\theta_1 < \theta$, and $\varphi \in X$, $\|T(z)\varphi\|$ is bounded in

$$\tilde{R}_{1,\theta_1} = \{z \,|\, |\arg z| \leq \theta_1, |z| \leq 1\}$$

so by the uniform boundedness principle, $\|T(z)\|$ is bounded in $\tilde{R}_{1,\theta_1}$. By using the semigroup property as above, one concludes from this that there are constants M, $\omega > 0$ so that

$$\|T(z)\| \leq Me^{\omega|z|}$$

for all $z \in \bar{S}_{\theta_1}$. Therefore, $e^{-\omega z}T(z)$ is a bounded holomorphic semigroup of angle θ_1. Notice that this is true for all $\theta_1 < \theta$ but ω will in general depend on θ_1. This characterization, Theorem X.52, and Corollary 2 above immediately yield:

Theorem X.53 A closed operator A on a Banach space X is the generator of a holomorphic semigroup of angle θ if and only if for all $\theta_1 < \theta$ there exist constants M, $\omega > 0$ so that $\lambda \notin \bar{S}_{\pi/2-\theta_1}$ implies that $\lambda - \omega \in \rho(A)$ and

$$\|(A - (\lambda - \omega))^{-1}\| \leq \frac{M}{\operatorname{dist}(\lambda, \bar{S}_{\pi/2-\theta_1})}$$

Furthermore, there exist constants M_0, $\omega_0 > 0$, so that for all $\varphi \in X$,

$$e^{-tA}\varphi \in \bigcap_{m=1}^{\infty} D(A^m) \quad \text{and} \quad \|A^m e^{-tA}\varphi\| \leq \frac{M_0 e^{\omega_0 t}\|\varphi\|}{t^m}$$

for all $t > 0$.

The proof of the following theorem closely parallels the proofs of Theorems X.12 and X.50 and is left to the reader (Problem 56).

Theorem X.54 Suppose that A is the generator of a holomorphic semigroup of angle θ on a Banach space X. Let B be a linear operator on X so that:

(i) $D(B) \supset D(A)$
(ii) For all $a > 0$, there is a $b > 0$ so that for all φ in $D(A)$

$$\|B\varphi\| \leq a\|A\varphi\| + b\|\varphi\|$$

Then $A + B$ on $D(A)$ is the generator of a holomorphic semigroup of angle θ.

To illustrate some of the concepts we have introduced and to show the use of holomorphic semigroups we discuss an example.

Example 5 (smoothness of solutions of the heat equation) We have previously shown (in Section IX.7) that the semigroup $e^{t\Delta}$ on $L^2(\mathbb{R}^n)$ may be represented by the formula

$$(e^{t\Delta}f)(x) = (4\pi t)^{-n/2}\int_{\mathbb{R}^n} e^{-|x-y|^2/4t} f(y)\,dy$$

By explicit computation, this formula also defines a strongly continuous semigroup on $C_\infty(\mathbb{R})$ whose infinitesimal generator on $\mathscr{S}(\mathbb{R})$ is $-\Delta$. Thus this is a representation for the semigroup $e^{t\Delta}$ on $C_\infty(\mathbb{R})$ which we constructed in Example 3.

For any $z \in \mathbb{C}$ with $\operatorname{Re} z > 0$, we define $e^{z\Delta}$ on $C_\infty(\mathbb{R}^n)$ by

$$(e^{z\Delta}f)(x) = (4\pi z)^{-n/2}\int_{\mathbb{R}^n} e^{-|x-y|^2/4z} f(y)\,dy$$

where we take the 1/2 root with the smallest argument. The reader can check by explicit computation (Problem 57) that $z \to e^{z\Delta}$ is an analytic operator-valued function for $\operatorname{Re} z > 0$, that the semigroup property holds, and that if $z \to 0$ in $\bar{S}_\theta$, $|\theta| < \pi/2$, then $e^{z\Delta}f \to f$. Furthermore,

$$\|e^{z\Delta}\| = \|(4\pi z)^{-n/2}e^{-|x|^2/4z}\|_1 = \frac{|z|}{\operatorname{Re} z}$$

so $e^{z\Delta}$ is a bounded holomorphic semigroup of angle $\pi/2$. Notice that if $z = te^{i\theta}$, $0 < |\theta| < \pi/2$, then $e^{te^{i\theta}\Delta}$ provides an example of a bounded semigroup that is not a contraction semigroup.

Suppose that $q(x)$ is a bounded continuous function. Then, by Theorem X.54, $-\Delta + q$, with domain $D(-\Delta)$, generates a holomorphic semigroup of angle $\pi/2$ on $C_\infty(\mathbb{R}^n)$. Further, for any $f \in C_\infty(\mathbb{R}^n)$, $e^{t(\Delta - q)}f \in \bigcap_{m=1}^\infty D((-\Delta + q)^m)$. If we suppose in addition that q is infinitely differentiable with bounded derivatives, then we can show that $e^{t(\Delta-q)}f$ is a C^∞ function of x for each $t > 0$. For let $\varphi \equiv e^{t(\Delta-q)}f$. Then $\varphi \in D((-\Delta + q)) = D(\Delta)$. Further, $\varphi \in D((-\Delta + q)^2)$, so $-\Delta\varphi + q\varphi \in D(\Delta)$. Since $\varphi \in D(\Delta)$, $\nabla\varphi$ is in $C_\infty(\mathbb{R}^n)$ by Problem 57b, and thus $q\varphi \in D(\Delta)$. It follows that $\Delta\varphi \in D(\Delta)$. Continuing in this way we prove that $\Delta^m\varphi \in D(\Delta)$ for all m. In particular, $\Delta^m\varphi$ is continuous for all m, so by Sobolev's lemma (Theorem IX.24) φ is a C^∞ function of x.

A similar proof shows that for $f \in L^2$, $e^{t(\Delta-q)}f$ is C^∞ in x for each $t > 0$. In this case we can conclude that $e^{t(\Delta-q)}f \in \bigcap_{m=1}^\infty D((-\Delta + q)^m)$ directly from the spectral theorem, so we do not need Theorem X.53.

By a simple argument using Sobolev's lemma and Theorem X.53, one can see that under the same hypotheses, the solutions,

$$u(x, t) = (e^{t(\Delta-q)}f)(x)$$

are C^∞ *jointly* in x and t for $t > 0$.

As a final example of the theory of holomorphic semigroups, we will investigate a class of operators which arise in the next section and later. Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and let A be a positive self-adjoint operator on $L^2(M, d\mu)$. Since $L^2 \subset L^p$ for all $1 \le p \le 2$, the contraction semigroup e^{-tA} is a densely defined map of L^p into L^p, $1 \le p \le 2$. The question naturally arises: Under what conditions can e^{-tA} be extended to a contraction semigroup on L^p.

Definition Let $\langle M, \mu\rangle$ be a σ-finite measure space and let A be a positive self-adjoint operator on $L^2(M, d\mu)$. We will call e^{-tA} an **L^p-contractive semigroup** if $\|e^{-tA}\varphi\|_p \le \|\varphi\|_p$ for all $\varphi \in L^2 \cap L^p$, *all* $p \in [1, \infty]$, and all $t > 0$. If the map $t \mapsto e^{-tA}$ is strongly continuous for all $p < \infty$ we will call e^{-tA} a **continuous** L^p-contractive semigroup.

Theorem X.55 Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and A a positive self-adjoint operator on $L^2(M, d\mu)$. Then

(a) If e^{-tA} is positivity preserving and $e^{-tA}1 = 1$, then e^{-tA} is an L^p-contractive semigroup.

(b) Every L^p-contractive semigroup is automatically continuous. Moreover, $\operatorname{Ker}(e^{-tA} \restriction L^p) = \{0\}$ for all $p > 1$ and $\operatorname{Ran}(e^{-tA} \restriction L^q)$ is dense in L^q for all $q < \infty$.

(c) Under the hypotheses of (a), for $1 < p < \infty$, e^{-tA} is a bounded holomorphic semigroup in the sector

$$S^{(p)} = \left\{ z \,\middle|\, |\arg z| < \frac{\pi}{2}\left(1 - \left|\frac{2}{p} - 1\right|\right)\right\}$$

Proof We begin by showing that e^{-tA} is a contraction on all the L^p spaces. First, suppose $f \in L^2$ and $f \ge 0$. Then

$$\|e^{-tA}f\|_1 = (1, e^{-tA}f) = (e^{-tA}1, f) = (1, f) = \|f\|_1$$

If $f \in L^2$ is real-valued, then we write $f = f_+ - f_-$ where $f_+ = \max\{0, f(x)\}$ and $f_- = \max\{0, -f(x)\}$. Then

$$\|e^{-tA}f\|_1 \le \|e^{-tA}f_+\|_1 + \|e^{-tA}f_-\|_1 = \|f_+\|_1 + \|f_-\|_1 = \|f\|_1$$

Finally, suppose $f(x) \in L^2$ is complex-valued. Then

$$\begin{aligned}|(e^{-tA}f)(x)| &= \sup_{\eta \text{ rational}} \{\mathrm{Re}[e^{-i\eta}(e^{-tA}f)(x)]\} \\ &= \sup_{\eta \text{ rational}} \{\mathrm{Re}[(e^{-tA}(e^{-i\eta}f))(x)]\} \\ &= \sup_{\eta \text{ rational}} \{(e^{-tA}(\mathrm{Re}\, e^{-i\eta}f))(x)\}\end{aligned}$$

for almost all x, where we have used the fact that e^{-tA} takes real functions into real functions since e^{-tA} is positivity preserving. Also, for each real $g \in L^2$,

$$\begin{aligned}|(e^{-tA}g)(x)| &= |e^{-tA}g_+ - e^{-tA}g_-| \\ &\le e^{-tA}g_+ + e^{-tA}g_- \\ &= e^{-tA}|g(x)|\end{aligned}$$

almost everywhere. Thus

$$|(e^{-tA}f)(x)| \le e^{-tA}|f(x)| \quad \text{a.e.} \tag{X.103}$$

which implies that $\|e^{-tA}f\|_1 \le \|e^{-tA}|f(x)|\|_1 = \|f\|_1$. Thus, for all $f \in L^2$, $\|e^{-tA}f\|_1 \le \|f\|_1$.

If $f \in L^\infty \subset L^2$, then

$$\begin{aligned}\|e^{-tA}f\|_\infty &= \sup_{\substack{\|g\|_1 = 1 \\ g \in L^2}} (e^{-tA}f, g) \\ &= \sup_{\substack{\|g\|_1 = 1 \\ g \in L^2}} (f, e^{-tA}g) \\ &\le \|f\|_\infty \left(\sup_{\|g\|_1 = 1} \|e^{-tA}g\|_1 \right) = \|f\|_\infty\end{aligned}$$

so e^{-tA} is a contraction on L^∞ also. Thus by the Riesz–Thorin theorem, e^{-tA} is a contraction on all the L^p spaces. To prove the analyticity statement, we need the Stein interpolation theorem (Theorem IX.21). Because A is positive and self-adjoint, $e^{-\zeta A}$ is analytic for $\mathrm{Re}\,\zeta > 0$, and continuous and bounded by one in the closed right half-plane as an operator on L^2. First, we interpolate between $p = 1$ and $p = 2$. Let $\eta > 0$ and $\theta \in (-\pi/2, \pi/2)$ be fixed. Then for all z satisfying $0 < \mathrm{Re}\, z < 1$, $e^{-\eta e^{i\theta z}A}$ is an analytic operator-valued function on $L^1 \cap L^2 = L^2$. Further, $e^{-\eta e^{i\theta z}A}$ is bounded and continuous on the closed strip $0 \le \mathrm{Re}\, z \le 1$. For $\mathrm{Re}\, z = 1$, $\|e^{-\eta e^{i\theta z}A}f\|_2 \le \|f\|_2$ and for $\mathrm{Re}\, z = 0$, $\|e^{-\eta e^{i\theta z}A}f\|_1 \le \|f\|_1$. Thus, by the Stein interpolation

theorem, for $t \in (0, 1)$, $\|e^{-\eta e^{i\theta t}A}f\|_p \le \|f\|_p$ where $t = 2 - 2/p$. Since $\eta > 0$ and $\theta \in (-\pi/2, \pi/2)$ were arbitrary, we conclude that

$$\|e^{-\zeta A}f\|_p \le \|f\|_p \qquad \text{whenever} \qquad |\arg \zeta| \le \frac{\pi}{2}\left(2 - \frac{2}{p}\right) = \frac{\pi}{2}\left(1 - \left|\frac{2}{p} - 1\right|\right)$$

The proof for $2 \le p < \infty$ is similar. Now, if f_k and g_k are simple functions, $\int_M (e^{-\zeta A}f_k)g_k\, d\mu$ is analytic in the right half-plane. If $f_k \xrightarrow{L^p} f$ and $g_k \xrightarrow{L^q} g$, where $p^{-1} + q^{-1} = 1$, then

$$\int_M (e^{-\zeta A}f_k)g_k\, d\mu \to \int_M (e^{-\zeta A}f)g\, d\mu$$

uniformly in $S^{(p)} = \{\zeta \,|\, |\arg \zeta| < (\pi/2)(1 - |(2/p) - 1|)\}$ so $\int_M (e^{-\zeta A}f)g\, d\mu$ is analytic in this sector. Since weakly analytic functions are strongly analytic (Theorem VI.4), $\zeta \to p^{-\zeta A}$ is analytic on $S^{(p)}$ as a function whose values are operators on L^p.

It remains to show that $e^{-zA}f \xrightarrow{L^p} f$ as $z \to 0$ in $S^{(p)}$ for each $f \in L^p$, $1 \le p < \infty$. If $z \in S^{(p)}$ and $1 \le p \le 2$, then $\|e^{-zA}f - f\|_p \le \|e^{-zA}f - f\|_2$ for $f \in L^2$. Since L^2 is dense in L^p, strong continuity follows since $\{e^{-zA}\}$ are uniformly bounded on L^p and e^{-zA} is strongly continuous on L^2. Now, suppose $2 < p < \infty$ and let q satisfy $p^{-1} + q^{-1} = 1$. Suppose that $e^{-t_0A}\psi = 0$ for some $\psi \in L^q$. Then $e^{-sA}\psi = 0$ for all $s \ge t_0$ and thus by analyticity $e^{-tA}\psi = 0$ for all $t > 0$. Since e^{-tA} is strongly continuous on L^q, $\psi = 0$. Thus $\mathrm{Ker}(e^{-tA}) = \{0\}$ on L^q for each $t > 0$. The reader can easily check that the adjoint of e^{-tA} on L^q is e^{-tA} on L^p. So we conclude that $\mathrm{Ran}(e^{-tA})$ is dense in L^p. Let $\psi = e^{-t_0A}\varphi$, $\varphi \in L^p$. Then

$$\|e^{-zA}\psi - \psi\|_p \le \|e^{-(z+t_0)A}\varphi - e^{-t_0A}\varphi\|_p \to 0$$

as $z \to 0$ by the analyticity in the interior of $S^{(p)}$ proved above. Since $\mathrm{Ran}(e^{-t_0A})$ is dense and the $\{e^{-zA}\}$ are uniformly bounded on $S^{(p)}$, we conclude that e^{-zA} is strongly continuous on L^p. ∎

There are examples where all the hypotheses of Theorem X.55 hold but where e^{-tA} is not strongly continuous on L^∞. In fact, the one-dimensional Hermite operator (Example 1 in Section X.7) provides such an example. For, in that case, $e^{-tA}\psi(x)$ is a continuous function of x for any $t > 0$ if $\psi \in L^\infty$, so $e^{-tA}\psi$ cannot converge in the L^∞-norm to ψ if ψ is not continuous.

X.9 Hypercontractive semigroups

In the previous section we discussed L^p-contractive semigroups. In this section we will prove a self-adjointness theorem for operators of the form $A + V$ where V is a multiplication operator and A generates an L^p-contractive semigroup that satisfies a strong additional property.

Definition Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and suppose that A is a positive self-adjoint operator on $L^2(M, d\mu)$. We say that e^{-tA} is a **hypercontractive semigroup** if:

(i) e^{-tA} is L^p-contractive;
(ii) for some $b > 2$ and some constant C_b, there is a $T > 0$ so that $\|e^{-TA}\varphi\|_b \leq C_b\|\varphi\|_2$ for all $\varphi \in L^2(M, d\mu)$.

By Theorem X.55, condition (i) implies that e^{-tA} is a strongly continuous contraction semigroup for all $p < \infty$. Hölder's inequality shows that

$$\|\cdot\|_q \leq \|\cdot\|_p \qquad \text{if} \quad p \geq q \tag{X.104}$$

Thus the L^p-spaces are a nested family of spaces which get smaller as p gets larger; this suggests that (ii) is a very strong condition. The following proposition shows that b plays no special role.

Proposition Let e^{-tA} be a hypercontractive semigroup on $L^2(M, d\mu)$. Then for all $p, q \in (1, \infty)$, there is a constant C_{pq} and a $t_{pq} > 0$ so that if $t \geq t_{pq}$ then

$$\|e^{-tA}\varphi\|_p \leq C_{pq}\|\varphi\|_q$$

for all $\varphi \in L^q$.

Proof The case where $p \leq q$ follows immediately from (i) and (X.104). So suppose that $p > q$. Since $e^{-TA}: L^2 \to L^b$ and $e^{-TA}: L^\infty \to L^\infty$, the Riesz–Thorin theorem implies that there is a constant C so that for all $r \geq 2$, $\|e^{-TA}\varphi\|_r \leq C\|\varphi\|_{br/2}$. We now consider two cases. First, if $q \geq 2$ we choose n large enough so that $2(b/2)^n > p$. Then $\|e^{-nTA}\varphi\|_{(b/2)^n 2} \leq C^n\|\varphi\|_2$, so the conclusion follows if $2 \leq q, p > 2(b/2)^n$, by using (X.104), and hypothesis (i). If $1 < q \leq 2$, then we choose n large enough so that $2(b/2)^n > p$ and $q > c$ where $c^{-1} + (2(b/2)^n)^{-1} = 1$. Since A is self-adjoint and $e^{-nTA}\varphi$ is a bounded map from L^2 to $L^{2(b/2)^n}$, $(e^{-nTA})^* = e^{-nTA}$ is a bounded map from L^c to L^2. Thus e^{-2nTA} is a bounded map from L^c to $L^{2(b/2)^n}$. Since $c < q < p < 2(b/2)^n$, (X.104) implies the proposition. ∎

Before proving the self-adjointness theorem, we present an example of a hypercontractive semigroup.

Example 1 We will use the terminology introduced in Example 2 of Section X.6. Let $U: L^2(\mathbb{R}) \to L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$ be the unitary map $U: f(x) \to \pi^{1/4}e^{x^2/2}f(x)$, and define $B = UNU^{-1}$. Then

$$B = -\frac{1}{2}\frac{d^2}{dx^2} + x\frac{d}{dx}$$

Since B is unitarily equivalent to N, B is essentially self-adjoint on the set of finite linear combinations of Hermite polynomials, $p_n(x) = U\phi_n$, B is positive, and $Bp_n = np_n$. Thus B generates a contraction semigroup e^{-tB} on $L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$. We will show that e^{-tB} is a hypercontractive semigroup.

Since $-d/dx^2$, $x^2 - 1$, and $-d^2/dx^2 + (x^2 - 1)$ are all essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, the Trotter product formula (Theorem X.51) implies that

$$e^{-tN}f = \lim_{n\to\infty}\left[\exp\left(\frac{t}{2n}\frac{d^2}{dx^2}\right)\exp\left(-\frac{t}{n}\left(\frac{1}{2}x^2 - 1\right)\right)\right]^n f$$

for all $f \in L^2(\mathbb{R}, dx)$. Since $\exp(-(t/n)(\frac{1}{2}x^2 - 1))$ and $\exp((t/2n)\,d^2/dx^2)$ (Problem 53) are positivity preserving, we conclude that e^{-tN} is positivity preserving. Since U is also positivity preserving, we have shown that e^{-tB} is positivity preserving. Further, $p_0(x) \equiv 1$ and $e^{-tB}p_0 = p_0$. Thus, by Theorem X.55, e^{-tB} is a semigroup of contractions on $L^p(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$ for each $p \in [1, \infty]$.

To prove hypercontractivity, we will show that $\|e^{-tB}\varphi\|_4 \leq C\|\varphi\|_2$ for t large enough. We begin by noticing that

$$\|p_n\|_{L^4(\mathbb{R}, \pi^{-1/2}e^{-x^2}dx)} = \left(\pi^{-1/2}\int_{-\infty}^{\infty}(p_n(x))^4 e^{-x^2}\,dx\right)^{1/4}$$

$$= \|p_n(x)\phi_n\|^{1/2}_{L^2(\mathbb{R}, dx)}$$

Now, since $A\phi_0 = 0$,

$$\phi_n(x) = (n!)^{-1/2}(A^\dagger)^n\phi_0 = (n!)^{-1/2}2^{n/2}{:}\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n{:}\phi_0$$

where the Wick power $:((A + A^\dagger)/\sqrt{2})^n:$ is defined by expanding and then moving all the $A^\dagger$ to the left in each term. Since $(A + A^\dagger)/\sqrt{2} = x$, the argument outlined in Problem 48 shows that the operator $:((A + A^\dagger)/\sqrt{2})^n:$

is just multiplication by a polynomial. But $\phi_n(x) = p_n(x)\phi_0$, so for any $\psi \in L^2(\mathbb{R}, dx)$,

$$p_n(x)\psi = 2^{n/2}(n!)^{-1/2}:\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n:\psi$$

Thus, using the estimate (X.61) we find that

$$\begin{aligned}\|p_n(x)\phi_n\|_{L^2(\mathbb{R}^n)} &= 2^{n/2}(n!)^{-1/2}\left\|:\left(\frac{A + A^\dagger}{\sqrt{2}}\right)^n:\phi_n\right\|_{L^2(\mathbb{R}^n)} \\ &\leq \frac{2^n}{(n!)^{1/2}}\left((n+1)^{1/2}\cdots(n+n)^{1/2}\right) \\ &= 2^n\left(\frac{(2n)!}{(n!)^2}\right)^{1/2} \\ &\leq 4^n\end{aligned}$$

Thus, if $\varphi = \sum_{n=0}^\infty a_n p_n(x) \in L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$, then

$$\begin{aligned}\left\|e^{-tB}\sum_{n=0}^\infty a_n p_n(x)\right\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)} &\leq \sum_{n=0}^\infty |a_n|e^{-tn}\|p_n(x)\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)} \\ &\leq \left(\sum_{n=0}^\infty |a_n|^2\right)^{1/2}\left(\sum_{n=0}^\infty e^{-2tn}4^n\right)^{1/2} \\ &\leq C\|\varphi\|_{L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)}\end{aligned}$$

for $t > \frac{1}{2}\log 4$. Therefore e^{-tB} is hypercontractive. We state the result as a theorem:

Theorem X.56 The operator $-\frac{1}{2}\,d^2/dx^2 + x\,d/dx$ on $L^2(\mathbb{R}, \pi^{-1/2}e^{-x^2}\,dx)$ is positive and essentially self-adjoint on the set of finite linear combinations of Hermite polynomials, and generates a hypercontractive semigroup.

As a preparation for our main theorem, we prove the following result. For generalizations, see the Notes.

Theorem X.57 (Segal's lemma) Let A and B be semibounded self-adjoint operators so that $A + B$ is essentially self-adjoint on $D(A) \cap D(B)$. Then

$$\|e^{-(A+B)}\| \leq \|e^{-A/2}e^{-B}e^{-A/2}\|$$

Proof Let $C = \|e^{-A/2}e^{-B}e^{-A/2}\|$. Let $\varphi \in Q(e^A)$. Then certainly

$$\varphi \in Q(e^{-B}) = \mathscr{H}$$

and

$$\begin{aligned}(\varphi, e^{-B}\varphi) &= (e^{A/2}\varphi, e^{-A/2}e^{-B}e^{-A/2}e^{A/2}\varphi) \\ &\leq C(\varphi, e^A\varphi)\end{aligned}$$

so we conclude that $\|e^{-B/2}\varphi\|^2 \leq C\|e^{A/2}\varphi\|^2$. It follows from Theorem X.18 that $(\varphi, e^{-B/2}\varphi) \leq (\varphi, C^{1/2}e^{-A/2}\varphi)$ or $\|e^{-B/4}\varphi\|^2 \leq C^{1/2}\|e^{A/4}\varphi\|^2$. By induction we have $\|e^{-2^{-n}B}\varphi\|^2 \leq C^{2^{1-n}}\|e^{2^{-n}A}\varphi\|^2$. Thus

$$(\varphi, e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}\varphi) \leq C^{2^{-n}}(\varphi, \varphi)$$

for all $\varphi \in Q(e^A)$. Since $e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}$ is a bounded self-adjoint operator,

$$\|e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A}\| \leq C^{2^{-n}}$$

so

$$\|(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n}\| \leq C$$

But by the Trotter product formula,

$$(e^{-2^{-(n+1)}A}e^{-2^{-n}B}e^{-2^{-(n+1)}A})^{2^n} \xrightarrow[n\to\infty]{} e^{-(A+B)}$$

strongly so $\|e^{-(A+B)}\| \leq C$ also. ∎

We are now ready to state our main theorem.

Theorem X.58 Let $\langle M, \mu\rangle$ be a measure space with $\mu(M) = 1$ and let H_0 be the generator of a hypercontractive semigroup on $L^2(M, d\mu)$. Let V be a real-valued measurable function on $\langle M, \mu\rangle$ such that $V \in L^p(M, d\mu)$ for all $p \in [1, \infty)$ and $e^{-tV} \in L^1(M, d\mu)$ for all $t > 0$. Then $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and is bounded below.

Proof The proof of the theorem is fairly long, so we will break it up into several steps. The idea is the following: First define

$$V_n(x) = \begin{cases} V(x) & \text{if } |V(x)| \leq n \\ 0 & \text{otherwise}\end{cases}$$

Then $H_n = H_0 + V_n$ is self-adjoint on $D(H_0)$ by the Kato–Rellich theorem. We will first derive various uniform bounds on e^{-tH_n} as a map from L^p to L^q. We then use these bounds to prove that e^{-tH_n} converges strongly to

a one-parameter self-adjoint semigroup $T(t)$ on $L^2(M, d\mu)$, so that $T(t)$ is generated by a semibounded self-adjoint operator H. Finally, we show that H is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and equals $H_0 + V$ there.

Step 1 *For any $t > 0$, $\sup_n \|e^{-tV_n}\|_1 < \infty$ and is uniformly bounded in t in any compact subinterval of $[0, \infty)$.*

To prove this statement, notice that if $V(x) < 0$, then $V_n(x) \geq V(x)$ so $e^{-tV_n(x)} \leq e^{-tV(x)}$. On the other hand, if $V(x) \geq 0$, then $V_n(x) \geq 0$ so that $e^{-tV_n(x)} \leq 1$. Thus, $e^{-tV_n(x)} \leq e^{-tV(x)} + 1$ for all x, so $\|e^{-tV_n(x)}\|_1 \leq \|e^{-tV}\|_1 + 1$. If

$$V_+(x) = \begin{cases} V(x), & V(x) \geq 0 \\ 0, & \text{otherwise} \end{cases}$$

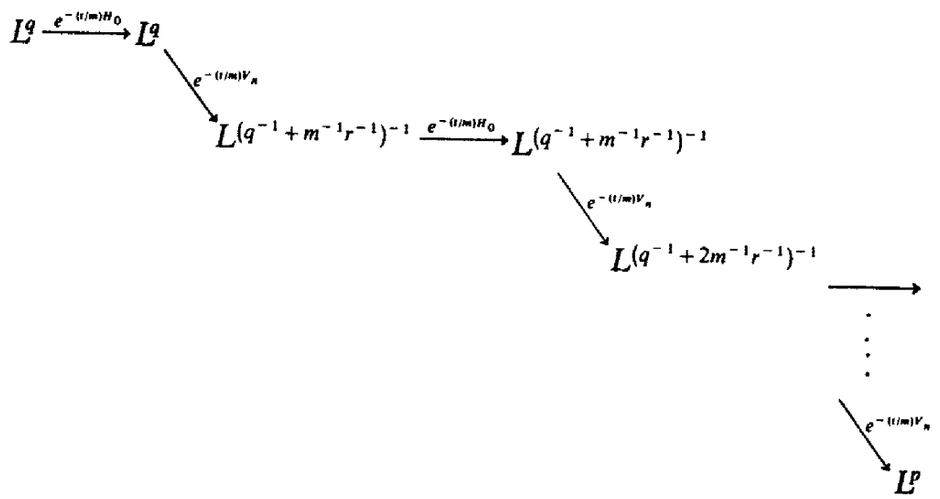
and $V_- = V - V_+$, then $\|e^{-tV_+}\|_1 \leq 1$ and $\|e^{-tV_-}\|_1$ is monotone increasing; the uniformity statement follows easily.

Step 2 *Let $p < q$ be given. Then for each t, there is a constant C_t (depending on q, p, and t but independent of n) so that for all $\varphi \in L^q$,*

$$\|e^{-tH_n}\varphi\|_p \leq C_t\|\varphi\|_q$$

For fixed p and q, C_t is uniformly bounded for t in a compact subinterval of $[0, \infty)$.

Notice that this is a fairly weak result since $p < q$, but the conditions on V are so strong that it will be sufficient when we need it in Step 4. Let $A_m = (e^{-tV_n/m}e^{-tH_0/m})^m$. We will first show that $\|A_m\varphi\|_p \leq C_t\|\varphi\|_q$ and then use the Trotter product formula. Let r satisfy $r^{-1} + q^{-1} = p^{-1}$. Then we can write the map A_m as



Each of the maps $e^{-(t/m)H_0}$ is a contraction since e^{-tH_0} is a hypercontractive semigroup. And by Hölder's inequality, each of the maps $e^{-(t/m)V_n}$ has norm less than or equal to $\|e^{-(t/m)V_n}\|_{mr}$. Thus

$$\|A_m\varphi\|_p \leq \|e^{-(t/m)V_n}\|_{mr}^m\|\varphi\|_q$$

Furthermore,

$$\|e^{-(t/m)V_n}\|_{mr}^m = \left[\left(\int_M e^{-tV_nr}\,d\mu\right)^{1/mr}\right]^m = \|e^{-tV_n}\|_r$$

so we conclude that

$$\|A_m\varphi\|_p \leq \|e^{-tV_n}\|_r\|\varphi\|_q$$

By the Trotter product formula $A_m\varphi \to e^{-tH_n}\varphi$ for all φ in L^2. But, by the weak-* compactness of the unit ball in L^p, $A_m\varphi$ also has a weak-* limit point ψ in L^p with $\|\psi\|_p \leq \|e^{-tV}\|_r\|\varphi\|_q$. A little measure theory now shows that we must have $\psi = e^{-tH_n}\varphi$. This proves the bound. The uniformity follows similarly to the uniformity in Step 1.

Step 3 *There is a constant E, independent of n, so that*

$$\|e^{-tH_n}\varphi\|_2 \leq e^{Et}\|\varphi\|_2$$

We first show that $e^{-TH_0}e^{-2TV_n}e^{-TH_0}$ is a bounded map from L^2 to L^2 with bound D independent of n. Since H_0 is hypercontractive, e^{-TH_0} is a bounded map (with bound D_1) from L^2 to L^4. By Hölder's inequality, e^{-2TV_n} is a bounded map from L^4 to L^2 with bound $\|e^{-2TV_n}\|_4 = \|e^{-8TV_n}\|_1^{1/4} \leq (\|e^{-8TV}\|_1 + 1)^{1/4}$ by Step 1. Finally, e^{-TH_0} is a contraction on L^2 so $\|e^{-TH_0}e^{-2TV_n}e^{-TH_0}\| \leq D$. Thus, by Segal's lemma,

$$\|e^{-2T(H_0+V_n)}\| \leq D$$

or

$$-E \equiv \frac{-\log D}{2T} \leq H_0 + V_n$$

Step 4 *Let $\varphi \in L^2(M, d\mu)$. Then $T(t)\varphi \equiv \lim_{n\to\infty} e^{-tH_n}\varphi$ exists and $T(t)$ is a strongly continuous semigroup of self-adjoint operators satisfying $\|T(t)\| \leq e^{Et}$. Further, there is a unique self-adjoint operator H satisfying $H \geq -E$ so that $T(t) = e^{-tH}$.*

We begin by expressing $e^{-tH_n}\varphi$ for $\varphi \in L^2$ by Duhamel's formula:

$$e^{-tH_n}\varphi = e^{-tH_m}\varphi + \int_0^t e^{-(t-u)H_n}(V_m - V_n)e^{-uH_m}\varphi\,du$$

This formula holds because both sides applied to a vector in $D(H_0)$ solve the same first order differential equation. Since H_n is self-adjoint on $D(H_0)$, the semigroups are equal. Now suppose $\varphi \in L^\infty$ and let t be fixed. Then by Step 2 we can find a constant K_1 so that $\|e^{-uH_n}\varphi\|_8 \leq K_1\|\varphi\|_\infty$ for all m and all $u \in [0, t]$. We can also find K_2 so that

$$\|e^{-(t-u)H_n}\psi\|_2 \leq K_2\|\psi\|_4$$

for all n and all $u \in [0, t]$. Finally, by Hölder's inequality, $V_m - V_n$ has norm $\|V_m - V_n\|_8$ as a map from L^8 to L^4. Thus by Duhamel's formula,

$$\|e^{-tH_n}\varphi - e^{-tH_m}\varphi\|_2 \leq K_1K_2\, t\|V_m - V_n\|_8\|\psi\|_\infty$$

Since $V_n \xrightarrow{L^8} V$, $e^{-tH_m}\varphi$ is Cauchy in L^2; so we can define $T(t)\varphi = \lim_{n\to\infty} e^{-tH_n}\varphi$. By Step 3, $\{e^{-tH_n}\}$ are uniformly bounded for t in compact subintervals of $[0, \infty)$ so an $\varepsilon/3$ argument shows that $e^{-tH_n}\varphi$ converges for all $\varphi \in L^2$. Similarly, since the convergence for $\varphi \in L^\infty$ is uniform on compact t intervals, $T(t)$ is a strongly continuous semigroup. We now define H to be the infinitesimal generator of $T(t)$. Since each e^{-tH} is self-adjoint, H is symmetric. But e^{-tH} is a semigroup bounded by e^{Et} so $-E - 1 \in \rho(H)$. By the fundamental criterion, H is self-adjoint. The bounds follow immediately from Step 3.

Step 5 *Let $\mathscr{D} = \{\varphi \mid \varphi = e^{-tH}\psi$ for some $\psi \in L^\infty\}$. Then, $\mathscr{D} \subset L^4 \cap D(H_0)$, H is essentially self-adjoint on $\mathscr{D}$, and if $\varphi \in \mathscr{D}$, $H\varphi = H_0\varphi + V\varphi$.*

L^∞ is dense in L^2, so by the spectral theorem, we know that $\mathscr{D}$ is dense in L^2. Also, by the spectral theorem, it is fairly easy to see that the set $(H + i)[\mathscr{D}]$ is L^2-dense, so H is essentially self-adjoint on $\mathscr{D}$. Now, suppose that $\varphi = e^{-tH}\psi \in \mathscr{D}$. By Step 2, $e^{-tH_n}\psi \in L^4$ and by using Duhamel's formula similarly to the above, one can show that $\{e^{-tH_n}\psi\}_{n=1}^\infty$ is Cauchy in L^4. Since $\varphi_n \equiv e^{-tH_n}\psi \xrightarrow{L^2} \varphi$ we conclude that $\varphi \in L^4 \subset D(V)$. Further, since $V_n \xrightarrow{L^4} V$, we have $V_n\varphi_n \xrightarrow{L^2} V\varphi$.

Now, let $f_n(t) = e^{-tH_n}$ and $f(t) = e^{-tH}$. Then $f_n(t)$ and $f(t)$ are analytic in the open right half-plane and by Step 3, $\|f_n(t)\| \leq e^{E(\mathrm{Re}\, t)}$ uniformly in n. Since $f_n(t) \to f(t)$ on the real axis, we conclude by the Vitali convergence theorem (Problem 33 of Chapter I) that $f_n(t) \to f(t)$ strongly, uniformly on compact subsets of the open right half-plane. It follows by the Cauchy integral theorem that $f_n'(t) \to f'(t)$ strongly, i.e.,

$$H_n\varphi_n \to H\varphi$$

Therefore,

$$H_0\varphi_n = (H_n - V_n)\varphi_n \to (H - V)\varphi$$

Thus, $\varphi \in D(H_0)$ and $H\varphi = H_0\varphi + V\varphi$.

Step 6 *$H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$.*

By Step 5, $H_0 + V$ is essentially self-adjoint on $D(H_0) \cap L^4$. Let $\psi \in D(H_0) \cap L^4$ and define $\psi_n = e^{-H_0/n}\psi$. Then by the spectral theorem $\psi_n \in C^\infty(H_0)$ and $H_0\psi_n \to H_0\psi$. But, since e^{-tH_0} is hypercontractive, $\psi_n \in L^4$ and $\psi_n \xrightarrow{L^4} \psi$. Thus, $V\psi_n \xrightarrow{L^2} V\psi$. Therefore

$$D(H_0) \cap L^4 \subset D(\overline{(H_0 + V) \restriction C^\infty(H_0) \cap L^4})$$

Since $L^4 \subset D(V)$, $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$.

This concludes the proof of Theorem X.58. ∎

We remark that if $V \geq 0$, then Step 1 and Step 3 (which uses Theorem X.57) are trivial. We have proven the more difficult theorem since in the main application that we have in mind (Example 4), V is not positive. Theorem X.58 has the following extension:

Theorem X.59 Let $\langle M, \mu\rangle$ be a finite measure space with $\mu(M) = 1$ and let H_0 be the self-adjoint generator of a hypercontractive semigroup on $L^2(M, d\mu)$. Assume that V is a real-valued measurable function on M which satisfies either:

(i) $V \in L^p$ for some $p > 2$ and $\|e^{-tV}\|_1 < \infty$ for all $t \geq 0$

or

(ii) $V \in L^2$ and $V \geq 0$.

Then $H_0 + V$ is essentially self-adjoint on $C^\infty(H_0) \cap D(V)$ and bounded below.

Finally, we state a continuity theorem which can be proven by the methods in the proof of Theorem X.58.

Theorem X.60 Let $\langle M, \mu\rangle$ be a finite measure space with $\mu(M) = 1$ and suppose that the self-adjoint operator H_0 generates a hypercontractive semigroup on $L^2(M, d\mu)$. Let $\{V_n\}_{n=1}^\infty$ and V be real-valued functions on M which satisfy:

(i) $V_n, V \in \bigcap_{p<\infty} L^p(M, d\mu)$

(ii) $e^{-V_n}, e^{-V} \in \bigcap_{p<\infty} L^p(M, d\mu)$

(iii) There is a $q \in (2, \infty]$ so that

$$V_n \xrightarrow{L^q} V \qquad \text{and} \qquad \sup_n \|e^{-V_n}\|_q < \infty$$

Then $H_0 + V_n \to H_0 + V$ in norm-resolvent sense.

Example 2 (the anharmonic oscillator, fourth proof) Let $V(x)$ be a non-negative measurable function on $\mathbb{R}$ which satisfies $\int_{-\infty}^{\infty} |V(x)|^p e^{-x^2}\, dx < \infty$ for all $p \in [1, \infty)$. Consider the operator $-d^2/dx^2 + 2x\, d/dx + (V(x) - 1)$ on the set $U[\mathscr{S}]$ where $U: L^2(\mathbb{R}) \to L^2(\mathbb{R}, \pi^{-1/2} e^{-x^2}\, dx)$ is the map defined in Example 1. In Example 1 we showed that $-d^2/dx^2 + 2x\, d/dx$ generates a hypercontractive semigroup. Thus, since $V(x) - 1$ satisfies the conditions of Theorem X.58, $-d^2/dx^2 + 2x\, d/dx + V(x) - 1$ is essentially self-adjoint on $U[\mathscr{S}]$. Therefore $-d^2/dx^2 + x^2 + V(x)$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$. In particular, if we take $V(x) = x^4$, we have another proof of the essential self-adjointness of the anharmonic oscillator on $\mathscr{S}(\mathbb{R})$.

Example 3 Let $V \in L^2(\mathbb{R}^n, \pi^{-n/2} e^{-|x|^2}\, d^n x)$ and $V \geq 0$. Theorem X.59 provides a proof that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ as follows: By generalizing Example 1, one shows that $-\Delta + 2x \cdot \nabla$ generates a hypercontractive semigroup on $L^2(\mathbb{R}^n, \pi^{-n/2} e^{-|x|^2}\, d^n x)$ so by Theorem X.59 and the method of Example 2, $-\Delta + x^2 + V$ is essentially self-adjoint on $C^\infty(-\Delta + x^2) \cap D(V) = \mathscr{S}(\mathbb{R}^n) \cap D(V)$. By a simple argument, it is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. Finally, as in Example 6 of Section X.2, one uses

$$[x_i, [x_j, -\Delta]] = \delta_{ij}$$

to prove that

$$\|x^2\psi\|^2 \leq \|(-\Delta + V + x^2)\psi\|^2 + 2n\|\psi\|^2$$

so by Konrady's trick, $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$. We have already proven this result in Section X.4 by using Kato's inequality.

Example 4 (application to quantum field theory) We will use the notation introduced in Section X.7.

Theorem X.61 Let $\mathscr{H}$ be a separable Hilbert space with complex conjugation C. Let A be a self-adjoint operator on $\mathscr{H}$ which commutes with C. Then

(a) If $A \geq 0$, then $\Gamma(e^{-tA})$ is an L^p-contractive semigroup on Q-space.
(b) If $A \geq cI > 0$, then $\Gamma(e^{-tA})$ is a hypercontractive semigroup.

Proof We will prove (a). The proof of (b) is essentially an infinite-dimensional version of the corresponding proof in Example 1 (see the Notes for a reference). Let A_n be a sequence of bounded self-adjoint operators whose spectra consist of finitely many eigenvalues of finite multiplicity so that $e^{-tA_n} \to e^{-tA}$ strongly as $n \to \infty$. Fix n, and let $\{a_\ell\}_{\ell=1}^N$ denote the non-zero eigenvalues of A_n with corresponding eigenfunctions $\{\psi_\ell\}_{\ell=1}^N$. Let $\{\psi_\ell\}_{\ell=N+1}^\infty$ be an orthonormal basis for the kernel of A_n. Let S be the unitary map of $\mathscr{F}_s(\mathscr{H})$ onto the Q space $L^2(Q, d\mu)$ constructed by using the basis $\{\psi_\ell\}_{\ell=1}^\infty$ for $\mathscr{H}$. We will show that SA_nS^{-1} is positivity preserving. If $\varphi(\cdot)$ and $\pi(\cdot)$ are the canonical field and conjugate momentum corresponding to C, then on the subspace $\{P(\varphi(\psi_\ell))\Omega_0 \mid P \text{ a polynomial}\}$ of $\mathscr{F}_s(\mathscr{H})$ the operator $d\Gamma(A_n)$ equals $\frac{1}{2}(\varphi(\psi_\ell)^2 + \pi(\psi_\ell)^2 - 1)$. Thus

$$Sd\Gamma(A_n)S^{-1} = \sum_{\ell=1}^N \frac{1}{2} a_\ell \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right)$$

Therefore,

$$S\Gamma(e^{-tA_n})S^{-1} = \prod_{\ell=1}^N \exp\left(-\frac{ta_\ell}{2} \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right) \right)$$

By Example 1, each $\exp(-(ta_\ell/2)(-d^2/dq_\ell^2 + 2q_\ell\, d/dq_\ell))$ is positivity preserving and

$$\exp\left(-\frac{ta_\ell}{2} \left(-\frac{d^2}{dq_\ell^2} + 2q_\ell \frac{d}{dq_\ell} \right) \right) 1 = 1$$

Thus, $S\Gamma(e^{-tA_n})S^{-1}$ is positivity preserving and $S\Gamma(e^{-tA_n})S^{-1}1 = 1$. Since e^{-tA_n} converges strongly to e^{-tA} on $\mathscr{H}$, $\Gamma(e^{-tA_n})$ converges strongly to $\Gamma(e^{-tA})$ on $\mathscr{F}_s(\mathscr{H})$. We conclude that $S\Gamma(e^{-tA})S^{-1}$ is positivity preserving and satisfies $S\Gamma(e^{-tA})S^{-1}1 = 1$. Therefore, by Theorem X.55, $S\Gamma(e^{-tA})S^{-1}$ is L^p-contractive. ∎

Corollary The free Hamiltonian $d\Gamma(\mu)$ of the free scalar field theory of mass $m > 0$ generates a hypercontractive semigroup $\Gamma(e^{-t\mu})$ on $\mathscr{F}_s(\mathscr{H})$.

Theorem X.62 The spatially cut-off Hamiltonian $H_0 + H_I(g)$ (defined in Section X.7) for a $(\varphi^4)_2$ self-interacting scalar field theory is essentially self-adjoint on $C^\infty(H_0) \cap D(H_I(g))$.

Proof Theorem X.45 and the above corollary show that SH_0S^{-1} and $SH_I(g)S^{-1}$ satisfy the hypotheses of Theorem X.58. ∎

X.10 Graph limits

In this section we continue the discussion of graph limits begun in Section VIII.7, using without comment the notation introduced there. In Theorem VIII.26 we showed that if $\{A_n\}_{n=1}^{\infty}$ *and* A are self-adjoint operators then $A_n \to A$ in the strong resolvent sense if and only if A is the strong graph limit of $\{A_n\}_{n=1}^{\infty}$. Although Theorem VIII.26 is interesting, it is not too useful since the proof depends heavily on the assumed existence of the self-adjoint limit A. In applications, it is often the self-adjointness of this limit which one is trying to establish. If we only assume that $(A_n + i)^{-1}$ and $(A_n - i)^{-1}$ converge strongly to operators R_+ and R_-, then the strong resolvent limit A exists if and only if either R_+ or R_- has dense range (Theorem VIII.22), a property which can be difficult to prove. On the other hand, the strong graph limit of a sequence of self-adjoint operators $\{A_n\}$ may exist but may not be self-adjoint, though it is automatically closed and symmetric (Theorem VIII.27). The point of the following theorem is that if *both* types of limit exist, then the limiting operator is self-adjoint. In fact, one need only use weak graph limits.

Theorem X.63 (graph limit theorem) Let $\{A_n\}_{n=1}^{\infty}$ be a sequence of self-adjoint operators on a Hilbert space $\mathscr{H}$. Suppose that:

(i) $(A_n \pm i)^{-1} \to R_{\pm}$ strongly

and

(ii) The weak graph limit A of $\{A_n\}_{n=1}^{\infty}$ is densely defined.

Then A is self-adjoint, $(A \pm i)^{-1} = R_{\pm}$, and A_n converges to A in strong resolvent sense.

Proof We first show that $\mathrm{Ker}(R_+) = \{0\}$. Let $\chi \in \mathrm{Ker}(R_+)$ and $\varphi \in D(A)$. Then there exists $\{\varphi_n\}_{n=1}^{\infty}$ with $\varphi_n \in D(A_n)$, $\varphi_n \to \varphi$, and $A_n\varphi_n \overset{w}{\to} A\varphi$. Thus

$$\begin{aligned}(\chi, \varphi) &= \lim_{n\to\infty} (\chi, \varphi_n)\\ &= \lim_{n\to\infty} ((A_n + i)^{-1}\chi, (A_n - i)\varphi_n)\\ &= (R_+\chi, A\varphi - i\varphi)\\ &= 0\end{aligned}$$

Since $D(A)$ is dense, $\chi = 0$. Thus $\mathrm{Ker}(R_+) = \{0\}$. Since $R_- = R_+^*$, $\mathrm{Ran}\, R_- = (\mathrm{Ker}\, R_+)^{\perp} = \mathscr{H}$. Therefore, by Theorem VIII.22, there is a self-adjoint operator A' so that $A_n \to A'$ in strong resolvent sense. Finally, Theorem VIII.26 implies that A' is the strong graph limit of $\{A_n\}$ so $A' \subset A$. But by Theorem VIII.28, A is symmetric, so $A' = A$. ∎

This theorem is important because it reduces the self-adjointness question to convergence questions, and these problems can sometimes be handled directly by estimates on the operators A_n. We will illustrate this with condition (i) first. Later we give a sufficient condition for (ii). How can one prove (i)? If $\varphi \in \mathscr{H}$, then *formally*

$$(A_n + i)^{-1}\varphi - (A_m + i)^{-1}\varphi = (A_n + i)^{-1}(A_n - A_m)(A_m + i)^{-1}\varphi \qquad \text{(X.105)}$$

This expression makes sense if $(A_m + i)^{-1}\varphi$ is both in $D(A_n)$ and $D(A_m)$. Thus, if m and n are fixed and we want (X.105) to hold for a dense set, we must require that $D_{n,m} \equiv (A_m + i)[D(A_n) \cap D(A_m)]$ be dense. Further if we want to take the limit of (X.105) for a fixed φ, we must require $\varphi \in \bigcap D_{n,m}$. Thus we cannot hope to use (X.105) unless $\bigcap D_{n,m}$ is dense. Once we have this regularity condition, then we can prove that the resolvents converge if both $A_n - A_m$ and $(A_m \pm i)^{-1}$ can be estimated uniformly in terms of an auxiliary self-adjoint operator:

Theorem X.64 Let $\{A_n\}$ be a sequence of self-adjoint operators with a common core D_0. Let N be a strictly positive self-adjoint operator so that for some $\alpha > 0$, $\beta > 0$:

(i) $\mathscr{D}^{\pm} = \bigcap_n (\mathrm{Ran}(A_n \pm i) \restriction D_0)$ are dense and $\mathscr{D}^{\pm} \subset D(N^{\alpha})$.
(ii) $\|N^{\beta}(A_n \pm i)^{-1}N^{-\alpha}\| \leq M$ for all n.
(iii) N^{β} is essentially self-adjoint on D_0 and

$$\|N^{-\beta}(A_n - A_m)N^{-\beta}\| \to 0 \qquad \text{as} \quad n, m \to \infty$$

Then, for each $\varphi \in \mathscr{H}$, $\{(A_n \pm i)^{-1}\varphi\}$ is a Cauchy sequence in $\mathscr{H}$.

Proof Let $\chi \in \mathscr{D}^+$ and define $\varphi_n = (A_n + i)^{-1}\chi$. Then

$$\begin{aligned}\|\varphi_n - \varphi_m\|^2 &= (\varphi_n - \varphi_m, \varphi_n - \varphi_m)\\ &= \mathrm{Im}(\varphi_n - \varphi_m, (A_n + i)(\varphi_n - \varphi_m))\\ &\leq |(\varphi_n - \varphi_m, (A_n + i)(\varphi_n - \varphi_m))|\\ &= |(\varphi_n - \varphi_m, (A_m - A_n)\varphi_m)|\\ &= |(N^{\beta}(\varphi_n - \varphi_m), N^{-\beta}(A_m - A_n)N^{-\beta}N^{\beta}\varphi_m)|\\ &\leq (2\sup_k \|N^{\beta}(A_k + i)^{-1}N^{-\alpha}N^{\alpha}\chi\|^2)\|N^{-\beta}(A_m - A_n)N^{-\beta}\|\\ &\leq 2M^2\|N^{\alpha}\chi\|^2\|N^{-\beta}(A_m - A_n)N^{-\beta}\|\\ &\to 0 \qquad \text{as} \quad n, m \to \infty\end{aligned}$$

Thus, $(A_n + i)^{-1}$ is strongly Cauchy on $\mathscr{D}^+$. Since $\mathscr{D}^+$ is dense and the $(A_n + i)^{-1}$ are uniformly bounded, $(A_n + i)^{-1}\varphi$ converges for all $\varphi \in \mathscr{H}$. The proof for $(A_n - i)^{-1}$ is the same. ∎

Example (the anharmonic oscillator, fifth proof) Let

$$H_0 = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right)$$

on $\mathscr{H} = L^2(\mathbb{R})$ and $V = x^4$. In the notation of Example 2 of Section X.6, $H_0 = A^\dagger A + \frac{1}{2}$ and $V = \frac{1}{4}(A + A^\dagger)^4$. Let E_n be the spectral projection of H_0 corresponding to the interval $[0, n]$. The range of E_n is finite dimensional and consists of the first n Hermite functions. We take D_0 to be the set of finite linear combinations of Hermite functions, set $A_n = H_0 + V_n$ where $V_n = E_n V E_n$, and $N = H_0$. We will show that A_n, N, and D_0 satisfy the hypotheses of Theorem X.64 with $\beta = 2$ and $\alpha = 1$. D_0 is a core for H_0, so since each $E_n V E_n$ is bounded, D_0 is a common core for $\{A_n\}_{n=1}^\infty$. To prove (i) notice that $\mathrm{Ran}[(A_n \pm i) \restriction (E_n \mathscr{H})] = E_n \mathscr{H}$ since A_n leaves $E_n \mathscr{H}$ invariant, $A_n \restriction E_n \mathscr{H}$ is self-adjoint, and $E_n \mathscr{H}$ is finite dimensional. On the other hand, the spectral theorem shows that $\mathrm{Ran}[(A_n \pm i) \restriction (D_0 \cap (I - E_n)\mathscr{H})] = D_0 \cap (I - E_n)\mathscr{H}$ since $A_n = H_0$ on $(I - E_n)\mathscr{H}$. Thus $\mathrm{Ran}(A_n \pm i) \restriction D_0 \supset D_0$. The converse inclusion holds trivially so we have $\mathscr{D}^\pm = \bigcap_n \mathrm{Ran}(A_n + i) \restriction D_0 = D_0$. Further, by the spectral theorem all powers of $N = H_0$ are essentially self-adjoint on D_0. The estimate in (iii) follows immediately from the fact that $V = \frac{1}{4}(A^\dagger + A)^4$ and the estimates (X.61). It remains to prove the estimate in (ii), i.e., that for $\varphi \in D_0$,

$$\|N^2(A_n \pm i)^{-1}N^{-1}\varphi\| \leq M\|\varphi\| \tag{X.106}$$

This is equivalent to showing that

$$N^4 \leq M_1(A_n \mp i)N^2(A_n \pm i) + M_2 \tag{X.107}$$

as quadratic forms on D_0. To prove (X.107) we expand:

$$\begin{aligned}(A_n \mp i)N^2(A_n \pm i) &= (N + V_n \mp i)N^2(N + V_n \pm i)\\ &= N^4 + V_n N^3 + N^3 V_n + (V_n \mp i)N^2(V_n \pm i)\\ &= N^4 + N^{3/2}V_n N^{3/2} + [N^{3/2}, [N^{3/2}, V_n]]\\ &\quad + (V_n \mp i)N^2(V_n \pm i)\\ &\geq N^4 + [N^{3/2}, [N^{3/2}, V_n]]\end{aligned} \tag{X.108}$$

since V_n and N are positive operators. Using the estimate (X.61) and the commutation properties of $A^\dagger$ and A, one can prove (Problem 62) that for any $\varepsilon > 0$, there is a b so that

$$\|[N^{3/2}, [N^{3/2}, V_n]]\varphi\| \leq \varepsilon\|N^4\varphi\| + b\|\varphi\|$$

for all $\varphi \in D_0$ and all n. Choosing ε small enough so that $2\varepsilon < 1$ we can conclude by Theorem X.18 that

$$[N^{3/2}, [N^{3/2}, V_n]] \leq 2\varepsilon N^4 + M_2 \tag{X.109}$$

as quadratic forms on D_0. Combining (X.108) and (X.109) we have (X.107), which proves the estimate in (ii).

We have thus verified that the hypotheses of Theorem X.64 hold for the sequence $H_0 + V_n$. Therefore, $(H + V_n \pm i)^{-1}$ converge strongly on $\mathscr{H}$. Furthermore, to apply Theorem X.63 we only need to show that $D^s_\infty = \{\psi \mid \langle\psi, \varphi\rangle \in \Gamma^s_\infty \text{ for some } \varphi\}$ is dense. In our case this is trivial since for all $\psi \in D_0$ we have $(H_0 + V_n)E_n\psi \to H_0\psi + x^4\psi$. Therefore by Theorem X.63, $H_0 + V_n$ converges in the strong resolvent sense to a self-adjoint operator C whose domain contains D_0 and $C \restriction D_0 = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4$.

This existence result is not particularly interesting since we could have immediately concluded from Theorem X.3 that $\frac{1}{2}(-d^2/dx^2 + x^2 + 2x^4) \restriction D_0$ has a self-adjoint extension. But, the following argument using the resolvent convergence allows us to prove self-adjointness on $D(H_0) \cap D(x^4)$. First we expand $(H_0 + V_n)^2$ finding that (as quadratic forms on D_0)

$$\begin{aligned}(H_0 + V_n)^2 &= H_0^2 + V_n^2 + H_0 V_n + V_n H_0\\ &= H_0^2 + V_n^2 + 2H_0^{1/2}V_n H_0^{1/2} + [H_0^{1/2}, [H_0^{1/2}, V_n]]\\ &\geq H_0^2 + V_n^2 + [H_0^{1/2}, [H_0^{1/2}, V_n]]\end{aligned}$$

since $V_n \geq 0$. A similar technique to the one outlined in Problem 62 to prove (X.109) can be used to prove that for any $\varepsilon > 0$ there is a constant b (independent of n) so that

$$0 \leq \varepsilon H_0^2 + [H_0^{1/2}, [H_0^{1/2}, V_n]] + b \tag{X.110}$$

Thus, there are constants c_1 and c_2 so that for $\varphi \in D_0$ and all n,

$$\|H_0\varphi\|^2 + \|V_n\varphi\|^2 \leq c_1\|(H_0 + V_n)\varphi\|^2 + c_2\|\varphi\|^2 \tag{X.111}$$

Now, let $\psi \in D(C)$. Then $\psi = (C + i)^{-1}\chi$ for some χ in $\mathscr{H}$. If we set $\psi_n = (H_0 + V_n + i)^{-1}\chi$, then $\psi_n \to \psi$. Thus, for each $\theta \in D_0$,

$$|(V\theta, \psi)| \leq \|V\theta\|\,\|\psi - \psi_n\| + \|(V - V_n)\theta\|\,\|\psi_n\| + |(\theta, V_n\psi_n)| \tag{X.112}$$

But from (X.111) it follows that

$$\begin{aligned}\|V_n\psi_n\| &\leq d_1\|(H_0 + V_n)\psi_n\| + d_2\|\psi_n\| \\ &\leq (d_1 + d_2)\|(H_0 + V_n + i)\psi_n\| = (d_1 + d_2)\|\chi\|\end{aligned}$$

Since the first two terms in (X.112) go to zero as $n \to \infty$, we conclude that $|(V\theta, \psi)| \leq (d_1 + d_2)\|\theta\|\ \|\chi\|$ for all $\theta \in D_0$. Thus $\psi \in D((V \upharpoonright D_0)^*) = D(V)$, so $D(C) \subset D(V)$. A similar proof shows that $D(C) \subset D(H_0)$. Therefore, $C = \frac{1}{2}(-d^2/dx^2 + x^2) + x^4$ is self-adjoint on $D(-d^2/dx^2 + x^2) \cap D(x^4)$.

This example gives the main ideas of the first self-adjointness proof for the spatially cut-off $(\varphi^4)_2$ Hamiltonian in quantum field theory. In the field theory case, the proofs of the estimates (X.109) and (X.110) are more difficult but use many of the same ideas (Problem 62).

We turn now to the problem of proving the condition (ii) of Theorem X.63. Since (ii) is sometimes difficult to verify directly, it is useful to have the following consequence of Theorem X.63. First, we make a definition.

Definition A sequence $\{A_n\}_{n=1}^{\infty}$ of positive self-adjoint operators is called **densely bounded** if there is a dense set $D_b \subset \mathscr{H}$ so that for any $\psi \in D_b$, there is a sequence $\{\psi_n\}_{n=1}^{\infty}$ so that

(i) $\psi_n \xrightarrow{\mathscr{H}} \psi$
(ii) $\psi_n \in Q(A_n)$
(iii) $\sup_n (\psi_n, A_n\psi_n) < \infty$

Theorem X.65 Let A_n be a sequence of positive self-adjoint operators on a Hilbert space $\mathscr{H}$. Suppose:

(i) $(A_n + 1)^{-1}$ converges to R strongly.
(ii) $\{A_n\}_{n=1}^{\infty}$ is densely bounded.

Then there is a self-adjoint operator A with $R = (A + 1)^{-1}$ so that $A_n \to A$ in strong resolvent sense.

Proof Let $B_n = (A_n + 1)^{1/2}$. Then $B_n^{-2} \to R$ strongly and since the B_n^{-2} are uniformly bounded positive operators, the continuity of the functional calculus for the square root (Theorem VIII.20 or Problem VI.14) implies that $B_n^{-1} \to R^{1/2}$ strongly. If we can show that there is a subsequence $\{B_{n_k}\}$ of $\{B_n\}$ so that the weak graph limit of $\{B_{n_k}\}$ is densely defined, then by a slight modification of Theorem X.63, we can conclude that $R^{1/2} = B^{-1}$ for some positive self-adjoint B. If we then set $A = B^2 - 1$, we have $R = (A + 1)^{-1}$ which proves the theorem.

We construct the subsequence of $\{B_n\}$ as follows. Let $\{\psi^{(k)}\}_{k=1}^{\infty}$ be a total set of vectors in D_b. Since $\{A_n\}_{n=1}^{\infty}$ is densely bounded, for each k we can find a sequence $\{\psi_n^{(k)}\}_{n=1}^{\infty}$ so that $\psi_n^{(k)} \in Q(A_n) = D(B_n)$, $\psi_n^{(k)} \to \psi^{(k)}$, and $\sup_n \|B_n\psi_n^{(k)}\| < \infty$. Now, consider the sequence $B_n\psi_n^{(1)}$. Since all the $B_n\psi_n^{(1)}$ are contained in a fixed ball in $\mathscr{H}$, we can find a weakly convergent subsequence $B_{n(1,j)}\psi_{n(1,j)}^{(1)}$ (because the balls are weakly sequentially compact). Similarly we choose a sequence $\psi_{n(1,j)}^{(2)} \to \psi^{(2)}$ and extract a subsequence of $B_{n(1,j)}$, call it $B_{n(2,j)}$, so that $B_{n(2,j)}\psi_{n(2,j)}^{(2)}$ is weakly convergent. We continue in this way and then (using the diagonalization trick) extract the subsequence $\{B_{n(j,j)}\}_{j=1}^{\infty}$ which has the property that for each k, there is a sequence $\psi_{n(j,j)}^{(k)}$ so that $\psi_{n(j,j)}^{(k)} \in D(B_{n(j,j)})$, $\psi_{n(j,j)}^{(k)} \to \psi^{(k)}$, and $B_{n(j,j)}\psi_{n(j,j)}^{k}$ converges weakly. Thus each $\psi^{(k)}$ is in D_∞^w for the sequence $B_{n(j,j)}$. Since D_b is dense and $\{\psi^{(k)}\}_{k=1}^{\infty}$ is total in D_b, D_∞^w is dense, which shows (by Theorem XIII.28) that the weak graph limit of the sequence $\{B_{n(j,j)}\}_{j=1}^{\infty}$ exists. ∎

This theorem has been applied to prove the existence of the spatially cut-off Hamiltonian in the Yukawa field theory in two dimensions. The details of the proof require the development of the free fermion field and several different sets of difficult estimates. Given the estimates, the idea is as follows: First, the interaction Hamiltonian $H(g, \kappa) = H_0 + H_I(g, \kappa)$ with both spatial and ultraviolet cut-offs is introduced. The spatial cut-off is similar to the spatial cut-off for the $(\varphi^4)_2$ field theory introduced in Section X.7. The ultraviolet cut-off means that the momentum space integral expressing H_I in terms of creation and annihilation operators is restricted to the region $|k| \leq \kappa$. Although $H(g, \kappa)$ makes sense on Fock space, $H(g, \kappa)$ "diverges" as $\kappa \to \infty$. A formal perturbation theory argument suggests that $H(g, \kappa)$ *should* diverge (!) because we have introduced the free field theory mass as an input parameter instead of the physically measurable interacting mass m and further because the free ground state should differ from the interacting ground state by an infinite amount of energy. The perturbation theory argument suggests that the "correct" Hamiltonian should be

$$H = H_0 + H_I - M - E \tag{X.113}$$

where E is given by a divergent integral and M is a well-defined operator multiplied by another divergent integral. Although H_I, M, and E are infinite on Fock space, H should be well defined because of cancellations. If we introduce spatial and momentum cut-off as described above, then

H_0, $H_I(g, \kappa)$, $M(g, \kappa)$, and $E(\kappa)$ are all finite and well defined on Fock space and

$$H_{\text{ren}}(g, \kappa) \equiv H_0 + H_I(g, \kappa) - M(g, \kappa) - E(\kappa)$$

is self-adjoint for each κ. Furthermore, it can be proven that $H_{\text{ren}}(g, \kappa)$ is bounded below uniformly in κ (say by C), that $(H_{\text{ren}}(g, \kappa) - C + 1)^{-1}$ converges strongly, and that $\{H_{\text{ren}}(g, \kappa)\}_{n=1}^{\infty}$ is densely bounded. Thus by Theorem X.65, $H_{\text{ren}}(g, \kappa)$ converges in norm resolvent sense to a self-adjoint operator $H(g)$. $H(g)$ is the "correct" spatially cut-off Hamiltonian. The spatial cut-off must be removed by other methods (see Chapter XIX).

X.11 The Feynman–Kac formula

Let H_0 be the free quantum mechanical Hamiltonian $-\Delta$ and let V be a potential so that $-\Delta + V$ is essentially self-adjoint on $D(-\Delta) \cap D(V)$. Then the Trotter product formula tells us how to express $e^{-it(H_0+V)}$ as a limit of products of $e^{-(it/n)H_0}$ and $e^{-(it/n)V}$ as $n \to \infty$. Since we have an explicit expression for e^{itH_0} as an integral operator (see (IX.31)),

$$(e^{-itH_0}f)(x) = \text{l.i.m.}(4\pi it)^{-3/2} \int_{\mathbb{R}^3} \exp\left(\frac{i|x-y|^2}{4t}\right) f(y)\, dy \qquad \text{(X.114)}$$

we can express $e^{-it(H_0+V)}$ as a limit of integral operators.

Theorem X.66 Let $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. Then

$$(e^{-it(H_0+V)}f)(x_0) = \lim_{n\to\infty} \left(\frac{4\pi it}{n}\right)^{-3n/2} \int_{\mathbb{R}^3} \cdots \int_{\mathbb{R}^3} \exp(iS_n(x_0, \ldots, x_n, t)) \times f(x_n)\, dx_n \cdots dx_1 \qquad \text{(X.115)}$$

where

$$S_n(x_0, x_1, \ldots, x_n, t) = \sum_{i=1}^{n} \frac{t}{n}\left[\frac{1}{4}\left(\frac{|x_i - x_{i-1}|}{t/n}\right)^2 - V(x_i)\right]$$

(All integrals taken in the sense $\int_{\mathbb{R}^3} = \lim_{m\to\infty} \int_{|x|\le m}$ and all limits taken in the L^2 sense.)

Proof Since $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, $H_0 + V$ is self-adjoint on $D(H_0)$ (Theorem X.15) and thus the Trotter product formula (Theorem VIII.30)

$$e^{-it(H_0+V)}f = \lim_{n\to\infty} (e^{-(it/n)H_0}e^{-(it/n)V})^n f$$

is applicable. The theorem follows by substituting the explicit expressions for $e^{-i(t/n)H_0}$ and $e^{-i(t/n)V}$. ∎

Formula (X.115) was stated by Feynman in 1948 on the basis of a physical interpretation. If a classical particle of mass m moves in a potential V, the smooth path $\omega(s)$, $0 \le s \le t$, is said to have **action** equal to

$$S(\omega) = \int_0^t \left(\frac{m}{2}|\dot\omega(s)|^2 - V(\omega(s))\right) ds \qquad \text{(X.116)}$$

The principle of least action of Lagrange says that the classical particle will travel the path of least action; i.e., the classical path will satisfy the Euler–Lagrange equation

$$m\ddot\omega(t) = -\nabla V(\omega(t))$$

corresponding to (X.116).

To see how to interpret (X.115) in terms of the action, take $m = \frac{1}{2}$ so that $H_0 = -(2m)^{-1}\Delta = -\Delta$. Given $x_0, x_1, \ldots, x_n$, consider a classical particle of mass $\frac{1}{2}$ moving along the polygonal path in Figure X.7 with constant velocity along each segment. The classical action of this path is

$$S(\omega) = \sum_{i=1}^{n} \left(\frac{t}{n}\right)\frac{1}{4}\left(\frac{|x_i - x_{i-1}|}{t/n}\right)^2 - \int_0^t V(\omega(t))\, dt$$

which approximately equals

$$S_n(x_0, x_1, \ldots, x_n, t) = \sum_{i=1}^{n} \left(\frac{t}{n}\right)\left[\frac{1}{4}\left(\frac{|x_i - x_{i-1}|}{t/n}\right)^2 - V(x_i)\right]$$

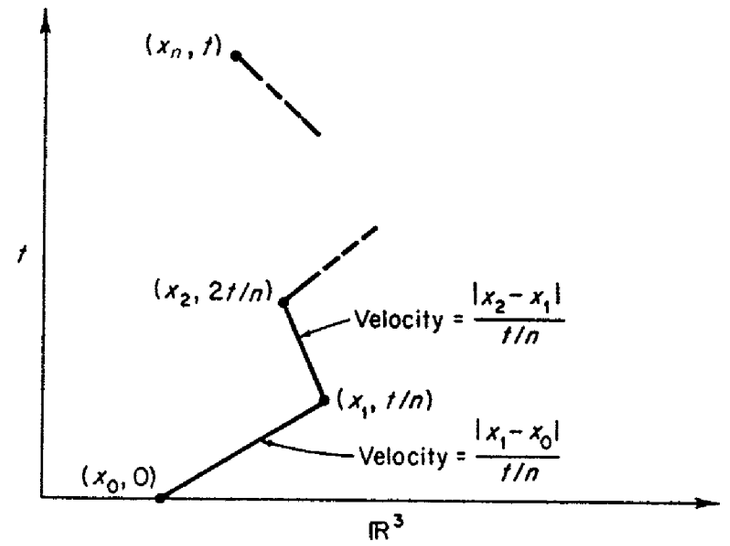


FIGURE X.7 A polygonal path between x_0 and x_n.

if V is continuous and the points $x_0, \ldots, x_n$ are close enough together. Thus

$$(4\pi it/n)^{-3n/2} \int \cdots \int e^{iS_n(x_0, \ldots, x_n, t)} f(x_n)\, dx_n\, dx_{n-1} \cdots dx_1$$

can be interpreted as an integral over all polygonal paths where S_n approximates the action of a classical particle moving along the path as indicated in Figure X.7. As $n \to \infty$, the set of polygonal paths becomes intuitively the set of all paths and given a path ω, $S_n(x_0, \ldots, x_n, t)$ approaches $S(\omega)$ if $\omega(0) = x_0$, $\omega(t) = x_n$, and the x_i lie on ω. Thus, intuitively, one can hope to find a formula for $(e^{-it(H_0+V)}f)(x_0)$ of the form

$$(e^{-it(H_0+V)}f)(x_0) = \int_{\Omega_{x_0}} e^{iS(\omega)} f(\omega(t))\, d\omega \tag{X.117}$$

where Ω_{x_0} is the set of all paths with $\omega(0) = x_0$, $S(\omega)$ is the classical action of the path ω, and $d\omega$ is a measure on Ω_{x_0}. In a natural way, the classical limit can be realized using this formula. If we put Planck's constant back in the Hamiltonian, then the formula reads

$$(e^{-it/\hbar(H_0+V)}f)(x_0) = \int_{\Omega_{x_0}} e^{iS(\omega)/\hbar} f(\omega(t))\, d\omega \tag{X.118}$$

As we take the classical limit by letting $\hbar$ go to zero, the oscillating phases in $e^{iS(\omega)/\hbar}$ tend to cancel except around paths where $S(\omega)$ is stationary. That is, most of the contribution to the dynamics comes from paths nearer and nearer to the classical paths as $\hbar \to 0$.

The above discussion shows why (X.117) is a beautiful heuristic formula. There is a mathematical notion of integration over paths introduced by Wiener, but unfortunately this notion *cannot* be used to make sense out of the right-hand side of (X.118). However, it can be used to derive an analogous formula for $(e^{-t(H_0+V)}f)(x_0)$ called the Feynman–Kac formula. Before proving this formula, we first need to discuss Wiener measure. Our construction of Wiener measure (using only our bare hands) is the most direct. We emphasize that there is an alternative approach using Gaussian random variables and the theory of Markov processes. This more natural approach provides an intuition which is invaluable for further developments, but introducing the necessary probabilistic machinery would take us too far afield. However, we feel that a discussion of the existence of dynamics would be incomplete without presenting the Feynman–Kac formula.

To motivate out construction of Wiener measure on $\mathbb{R}^n$ notice that the Trotter product formula implies that for suitable V,

$$e^{-t(H_0+V)}f = \lim_{m\to\infty} (e^{-(t/m)H_0}e^{-(t/m)V})^m f$$

with

$$(e^{-(t/m)H_0}e^{-(t/m)V})^m f = \int \cdots \int p\left(x_0, x_1; \frac{t}{m}\right) e^{-(t/m)V(x_1)} \cdots$$

$$\times\, p\left(x_{m-1}, x_m; \frac{t}{m}\right) e^{-(t/m)V(x_m)} f(x_m)\, dx_1 \cdots dx_m \tag{X.119}$$

where

$$p(x, y; t) = (4\pi t)^{-n/2} e^{-|x-y|^2/4t}$$

There are two problems in trying to take m to infinity in the right-hand side of (X.119). The first is that the infinite product of Lebesgue measures does not yield a reasonable measure. Secondly, the product of the kernels p intuitively approaches

$$\exp\left(-\int \dot{\omega}(t)^2\, dt\right) \tag{X.120}$$

and for arbitrary paths $\dot{\omega}(t)$ is very singular. Fortunately, these two difficulties cancel so long as we lump the two terms together. Thus, our plan is to try to construct a measure μ_{x_0} on a space of paths starting at x_0 so that the right-hand side of (X.119) is just equal to

$$\int_\Omega \prod_{j=1}^{m} e^{-(t/m)V(\omega(jt/m))}\, d\mu_{x_0}(\omega) \tag{X.121}$$

Since the "zero" of (X.120) will be used to cancel the "infinity" of the infinite product of Lebesgue measures, one should not be surprised that this procedure does not work if (X.120) is replaced by $\exp(-i\int \dot{\omega}(t)^2\, dt)$. This is in fact the case (Problem 64). With this motivation, we begin our construction.

Let $\dot{\mathbb{R}}^n$ be the one point compactification of $\mathbb{R}^n$ and let $\Omega = \bigtimes_{0\le t} \dot{\mathbb{R}}^n$, the product of uncountably many copies of $\dot{\mathbb{R}}^n$. Then Ω is just the set of all paths in $\dot{\mathbb{R}}^n$ for $t \ge 0$; these are just the paths in $\mathbb{R}^n$ except that they may pass through infinity. We will always consider Ω with the product topology under which it is a compact Hausdorff space by the Tychonoff theorem. This space is so big that the Borel and Baire sets differ. We will always consider regular Borel measures. Now, let $F(x_1, \ldots, x_m)$ be a continuous function on $\bigtimes_{j=1}^m \dot{\mathbb{R}}^n$ and fix $t_1 \le \cdots \le t_m$. Then, $\varphi(\omega) = F(\omega(t_1), \ldots, \omega(t_m))$ is a continuous function on Ω. We denote the set of such continuous functions on Ω, for arbitrary m, by $C_{\text{fin}}(\Omega)$ and for such φ we *define*

$$L_{x_0}(\varphi) = \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} F(x_1, \ldots, x_m) p(x_0, x_1; t_1) p(x_1, x_2; t_2 - t_1) \cdots$$
$$\times\, p(x_{m-1}, x_m; t_m - t_{m-1})\, dx_1 \cdots dx_m \tag{X.122}$$

L_{x_0} is a well-defined linear functional on $C_{\text{fin}}(\Omega)$ because if F does not depend on x_k, we can use the semigroup property of the heat equation:

$$\int_{\mathbb{R}^n} p(x_{k-1}, x_k\,; t_k - t_{k-1}) p(x_k, x_{k+1}; t_{k+1} - t_k)\, dx_k$$

$$= p(x_{k-1}, x_{k+1}; t_{k+1} - t_{k-1})$$

to integrate out the variable x_k. Thus $L_{x_0}(\varphi)$ is independent of the representation of φ. Further, $L_{x_0}(1) = 1$ and $L_{x_0}(\varphi) \geq 0$ if $\varphi \geq 0$ since p is positive. Therefore, by the proposition before Theorem IV.14,

$$|L_{x_0}(\varphi)| \leq \sup_{\omega \in \Omega} |\varphi(\omega)|$$

So L_{x_0} is a positive linear functional of norm one on $C_{\text{fin}}(\Omega)$. But, by the Stone–Weierstrass theorem, $C_{\text{fin}}(\Omega)$ is dense in $C(\Omega)$, so L_{x_0} has a unique extension (which we also denote by L_{x_0}) to a positive linear functional of norm one on $C(\Omega)$. Finally, by the Riesz–Markov theorem there is a unique regular Borel measure μ_{x_0} on Ω with $\mu_{x_0}(\Omega) = 1$ so that

$$L_{x_0}(\varphi) = \int_\Omega \varphi\, d\mu_{x_0} \qquad \text{for all} \quad \varphi \in C(\Omega)$$

For each x_0, μ_{x_0} is called a **Wiener measure** on Ω and sometimes the whole family of measures $\{\mu_x \mid x \in \mathbb{R}^n\}$ is called Wiener measure.

The measure that we have constructed is a Borel measure. Many interesting sets of paths are Borel subsets of Ω, for example:

Lemma For $0 < \alpha \leq 1$, the set Ω_α of Hölder continuous paths of order α is a Borel subset of Ω.

Proof A path ω is in Ω_α if and only if for all $m < \infty$ there is an M so that

$$|\omega(s) - \omega(t)| \leq M|s - t|^\alpha, \qquad 0 \leq s, t \leq m$$

Therefore,

$$\Omega_\alpha = \bigcap_{m=1}^{\infty} \bigcup_{n=1}^{\infty} \bigcap_{0 \leq s,\, t \leq m} \{\omega \,|\, |\omega(s) - \omega(t)| \leq n|s - t|^\alpha\}$$

Since $\{\omega \,|\, |\omega(s) - \omega(t)| \leq n|s - t|^\alpha\}$ is closed and arbitrary intersections of closed sets are closed, Ω_α is Borel because the last two operations are countable. ∎

The following theorem assures us that the measure μ_{x_0} constructed on the unreasonably large space Ω has support on a set of continuous paths although not on the set of continuously differentiable paths. For a reference, see the Notes.

Theorem X.67 If $0 < \alpha < \frac{1}{2}$, then $\mu_{x_0}(\Omega_\alpha) = 1$ for all $x_0 \in \mathbb{R}^n$. If $\frac{1}{2} \leq \alpha \leq 1$, then $\mu_{x_0}(\Omega_\alpha) = 0$ for all $x_0 \in \mathbb{R}^n$.

We have stated Theorem X.67 because it is used in the proof of the following lemma outlined in Problem 65:

Lemma Let S be a Borel set of Lebesgue measure zero in $\mathbb{R}^n$ and let Ω_S be the set of paths in Ω_α so that $\{t \,|\, \omega(t) \in S\}$ has Lebesgue measure zero. Then, for each x in $\mathbb{R}^n$, $\mu_x\{\Omega_S\} = 1$.

We now return to our discussion of the semigroups e^{-tH_0} and $e^{-t(H_0+V)}$. By our construction of μ_x we know that for each continuous function f on $\mathbb{R}^n$, we have, for fixed $\alpha \in (0, \frac{1}{2})$,

$$\int_{\Omega_\alpha} f(\omega(t))\, d\mu_x(\omega) = \int_{\mathbb{R}^n} f(y) p(x, y; t)\, dy \tag{X.123}$$

If f is any measurable function on $\mathbb{R}^n$ so that $f(\cdot)p(x, \cdot, t)$ is integrable, we can approximate f by continuous functions. Then, an application of the dominated convergence theorem shows that (X.123) holds for such f. In particular, (X.123) holds for all $f \in L^2(\mathbb{R}^n)$. But by (IX.31), the right-hand side of (X.123) is just $(e^{-tH_0}f)(x)$, so we have

$$(e^{-tH_0}f)(x) = \int_\Omega f(\omega(t))\, d\mu_x(\omega) \qquad \text{for all } f \in L^2(\mathbb{R}^n)$$

This is the path space integral which gives the free semigroup. We state our interacting path space formulae on $\mathbb{R}^3$. By changing L^2 to L^p with $p > n/2$, it is easy to obtain Feynman–Kac formulae on $\mathbb{R}^n$.

Theorem X.68 (the Feynman–Kac formula) Let V be a real-valued function in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and let $H = H_0 + V$ where $H_0 = -\Delta$. Then for all $f \in L^2(\mathbb{R}^3)$,

$$(e^{-tH}f)(x) = \int_{\Omega_\alpha} f(\omega(t)) \exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_x(\omega) \tag{X.124}$$

Proof We prove the theorem in four steps: first for continuous V of compact support, second for V in $L^\infty(\mathbb{R}^3)$, third for $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $V \leq 0$, and finally for V in the general case. So suppose V is continuous

with compact support. Using (X.119) and (X.122), we have

$$\begin{aligned}[(e^{-(t/m)H_0}e^{-(t/m)V})^m f](x) &= \int_{\mathbb{R}^3}\cdots\int_{\mathbb{R}^3} p\left(x, x_m; \frac{t}{m}\right)\cdots p\left(x_2, x_1; \frac{t}{m}\right) \\ &\quad \times f(x_1)\exp\left(-\sum_{j=1}^{m}\frac{t}{m}V(x_j)\right) dx_1\cdots dx_m \\ &= \int_{\Omega_x}\exp\left(-\frac{t}{m}\sum_{j=1}^{m}V\left(\omega\left(\frac{jt}{m}\right)\right)\right) f(\omega(t))\, d\mu_x(\omega) \qquad \text{(X.125)}\end{aligned}$$

By the hypotheses on V, $H_0 + V$ is self-adjoint on $D(H_0) = D(H_0) \cap D(V)$, so by the Trotter product formula, $(e^{-(t/m)H_0}e^{-(t/m)V})^m f$ converges to $e^{-tH}f$ in $L^2(\mathbb{R}^3)$. Therefore, there is a subsequence $\{m_j\}$ so that $(e^{-(t/m_j)H_0}e^{-(t/m_j)V})^{m_j} f$ converges to $e^{-tH}f$ almost everywhere. On the other hand, if ω is a continuous path, then $V(\omega(t))$ is continuous in t so

$$\frac{t}{m}\sum_{j=1}^{m}V\left(\omega\left(\frac{jt}{m}\right)\right) \to \int_0^t V(\omega(s))\, ds$$

as $m \to \infty$. Since for each x, almost all (with respect to μ_x) paths are continuous,

$$f(\omega(t))\exp\left(-\frac{t}{n}\sum_{j=1}^{n}V\left(\omega\left(\frac{jt}{n}\right)\right)\right) \to f(\omega(t))\exp\left(-\int_0^t V(\omega(s))\, ds\right)$$

pointwise almost everywhere on Ω_α as $m \to \infty$. Furthermore,

$$\begin{aligned}\int_{\Omega_x}\left| f(\omega(t))\exp\left(-\frac{t}{n}\sum_{j=1}^{n}V\left(\omega\left(\frac{jt}{n}\right)\right)\right)\right| d\mu_x(\omega) &\le e^{t\max|V|}\int_{\Omega_x}|f(\omega(t))|\, d\mu_x(\omega) \\ &= e^{t\max|V|}(e^{-tH_0}|f|)(x) \\ &< \infty\end{aligned}$$

for almost all x. Therefore, by the dominated convergence theorem, the right-hand side of (X.125) converges to

$$\int_\Omega f(\omega(t))\exp\left(-\int_0^t V(\omega(s))\, ds\right) d\mu_x(\omega)$$

for almost all x. This proves (X.124) under the special hypotheses that V is continuous with compact support.

Now, suppose that $V \in L^\infty(\mathbb{R}^3)$ and let V_n be a sequence of continuous functions of compact support so that $|V_n(x)| \le \|V\|_\infty$ for all x and $V_n(x) \to V(x)$ pointwise a.e. Then $(H_0 + V_n)$ converges to $H_0 + V$ in strong resolvent sense, so by Theorem VIII.20, $e^{-t(H_0+V_n)}$ converges strongly to $e^{-t(H_0+V)}$ for each $t \ge 0$. By step one,

$$(e^{-t(H_0+V_n)}f)(x) = \int_{\Omega_x} f(\omega(t))\exp\left(-\int_0^t V_n(\omega(s))\, ds\right) d\mu_x(\omega) \qquad \text{(X.126)}$$

for almost all x and all n. Since $V_n \to V$ pointwise a.e., the lemma implies that for almost all $\omega \in \Omega_\alpha$, $V_n(\omega(t)) \to V(\omega(t))$ pointwise a.e. in t. Therefore, since the V_n and V are uniformly bounded, we have $\int_0^t V_n(\omega(s))\, ds \to \int_0^t V(\omega(s))\, ds$ pointwise a.e. on Ω_α. Thus

$$f(\omega(t))\exp\left(-\int_0^t V_n(\omega(s))\, ds\right) \to f(\omega(t))\exp\left(-\int_0^t V(\omega(s))\, ds\right)$$

pointwise a.e. on Ω_α, and now the same dominated convergence theorem argument as in step one shows that the right-hand side of (X.126) converges to the right-hand side of (X.124). On the other hand, as before, a subsequence of the left-hand side of (X.126) converges pointwise a.e. to $e^{-t(H_0+V)}f$ because of the strong convergence. Thus, (X.124) holds in the second case.

Now, suppose that $V \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $V \le 0$. Let $V_n(x) = \max\{V(x), -n\}$. Then V_n is a sequence of decreasing L^∞ functions so that $V_n \xrightarrow{L^2+L^\infty} V$ and $V_n \to V$ pointwise a.e. For each n, the formula (X.124) holds and as $n \to \infty$, $\int_0^t V_n(\omega(s))\, ds \to \int_0^t V(\omega(s))\, ds$ a.e. on Ω_α by the lemma and the monotone convergence theorem. The proof is completed by appealing to the argument in the second case and the monotone convergence theorem.

By obvious modification, the third case holds for V bounded from above and so, appealing again to the monotone convergence theorem, we conclude the proof in the general case. ∎

If $V \in L^2 + (L^\infty)$, then the Feynman–Kac formula implies that

$$\int_\Omega \exp\left(-\int_0^t V(\omega(s))\, ds\right) f(\omega(t))\, d\mu_x(\omega) < \infty$$

for almost all $x \in \mathbb{R}^n$. Therefore

$$-\int_0^t V(\omega(s))\, ds < \infty$$

for almost all ω, for almost all x. Since we can write an arbitrary $V \in L^2 + (L^\infty)$ as a linear combination of its positive and negative parts, we conclude that

$$\int_0^t |V(\omega(s))|\, ds < \infty$$

for almost all ω, for almost all x, if $V \in L^2 + (L^\infty)$.

X.12 Time-dependent Hamiltonians

In this section we prove two existence theorems for the time-dependent Schrödinger equation

$$\frac{d\varphi(t)}{dt} = -iH(t)\varphi(t) \tag{X.127}$$

The investigation of time-dependent problems is important because one sometimes wants to calculate the change in a quantum system in a variety of situations, for example, when an external potential is turned on and then switched off after a short time or when a periodic potential is turned on. We first introduce the analogue of unitary one-parameter groups.

Definition A two-parameter family of unitary operators $U(s, t)$, $s, t \in \mathbb{R}$ which satisfies:

(a) $U(r, s)U(s, t) = U(r, t)$
(b) $U(t, t) = I$
(c) $U(s, t)$ is jointly strongly continuous in s and t

is called a **unitary propagator**.

Theorem X.69 (the Dyson expansion) Let $t \to H(t)$ be a strongly continuous map of $\mathbb{R}$ into the *bounded* self-adjoint operators on a Hilbert space $\mathscr{H}$. Then there is a unitary propagator on $\mathscr{H}$ so that, for all $\psi \in \mathscr{H}$,

$$\varphi_s(t) = U(t, s)\psi$$

satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.128}$$

Proof We define

$$U(t, s)\varphi = 1 + \sum_{n=1}^{\infty} (-i)^n \int_s^t \int_s^{t_1} \cdots \int_s^{t_{n-1}} H(t_1) \cdots H(t_n)\varphi \, dt_n \cdots dt_1 \tag{X.129}$$

By the uniform boundedness principle, $H(\tau)$ is uniformly bounded on $[s, t]$, so the nth term on the right is bounded by

$$\frac{|t-s|^n}{n!}\left(\sup_{\tau \in [s,t]} \|H(\tau)\|\right)^n \|\varphi\|$$

so the series on the right converges in the uniform operator topology to $U(t, s)$. Thus $U(t, s)$ is jointly strongly continuous in s and t since this is true of each term on the right. It is trivial to check that $U(t, t) = I$ and that $U(t, s)^* = U(s, t)$; the formula $U(r, s)U(s, t) = U(r, t)$ is proven by multiplying out the series as in the case of unitary groups generated by bounded operators. Thus,

$$U(s, t)U(s, t)^* = I = U(s, t)^*U(s, t)$$

so $U(t, s)$ is unitary. The first statement in (X.128) follows by differentiating the series for $U(t, s)$ term by term and noting that the resulting series converges uniformly. ∎

We remark that the self-adjointness of the $H(t)$ was used only in proving that $U(t, s)$ is unitary; without self-adjointness we can still define $U(t, s)$ as before and use it to construct strong solutions $\varphi_s(t)$.

Although the Dyson expansion requires that $H(t)$ be bounded, by passing to the "interaction representation" we can use it to handle certain cases of the form

$$H(t) = H_0 + V(t)$$

where H_0 is a (possibly unbounded) self-adjoint operator and $t \to V(t)$ satisfies the hypotheses of Theorem X.69. Define

$$\tilde{V}(t) = e^{iH_0t}V(t)e^{-iH_0t}$$

Then $t \to \tilde{V}(t)$ also satisfies the hypotheses of Theorem X.69; we denote the corresponding propagator by $\tilde{U}(t, s)$. If we now set

$$U(t, s) = e^{-itH_0}\tilde{U}(t, s)e^{isH_0}$$

then, at least *formally*, $U(t, s)$ satisfies

$$\frac{d}{dt}U(t, s) = -iH_0 e^{-itH_0}\tilde{U}(t, s)e^{isH_0} + e^{-itH_0}(-i\tilde{V}(t))\tilde{U}(t, s)e^{isH_0}$$

$$= (-iH_0 - iV(t))U(t, s)$$

so $\varphi_s(t) = U(t, s)\psi$ should be a strong solution of

$$\frac{d}{dt}\varphi_s(t) = -i(H_0 + V(t))\varphi_s(t), \qquad \varphi_s(s) = \psi$$

The difficulty is that $H_0 U(t, s)\psi = H_0 e^{-itH_0}\tilde{U}(t, s)e^{isH_0}\psi$ may not make sense since $\tilde{U}(t, s)\psi$ may not be in the domain of H_0 even if ψ is. It can be shown (Problem 66) that if $t \to [H_0, V(t)]$ is strongly continuous, then

$\varphi_s(t)$ is in fact a strong solution. This hypothesis is a special case of the more general hypotheses in Theorem X.70 (below); these give rise to strong solutions, so we will not pursue this problem further here. However, we note that for any $\psi \in \mathscr{H}$, $\psi_s(t) = e^{-iH_0 t}\tilde{U}(t, s)e^{isH_0}\psi$ is always a "weak" solution in the sense that for any $\eta \in D(H_0)$, $(\eta, \psi_s(t))$ is differentiable and

$$\frac{d}{dt}(\eta, \psi_s(t)) = -i(H_0\eta, \psi_s(t)) - i(V(t)\eta, \psi_s(t))$$

Example 1 The Dyson expansion is important for practical calculations also. Suppose that H_0 is the Hamiltonian of a quantum system and that ψ_k and ψ_ℓ are eigenfunctions of H_0 with corresponding eigenvalues λ_k and λ_ℓ. If the system starts out in state ψ_k, it will stay in ψ_k in the absence of any external potential since $e^{itH_0}\psi_k = e^{it\lambda_k}\psi_k$. However, if an external potential $V(t)$ is turned on for a while the dynamics is given by $e^{-itH_0}\tilde{U}(t, 0)\psi_k$, and if we look at the system at time t the probability that the system will be observed in state ψ_ℓ is $|(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k)|^2$, the transition probability from ψ_k to ψ_ℓ. Using the Dyson expansion we have

$$(\psi_\ell, e^{-itH_0}\tilde{U}(t, 0)\psi_k) = (\psi_\ell, e^{-itH_0}\psi_k) - i\int_0^t (\psi_\ell, e^{-iH_0 t}\tilde{V}(t_1)\psi_k)\, dt_1 + \cdots$$

$$= -i\int_0^t e^{-i\lambda_\ell t}e^{-i(\lambda_k - \lambda_\ell)t_1}(\psi_\ell, V(t_1)\psi_k)\, dt_1 + O(t^2)$$

The constant in the term of order t^2 can be easily bounded by estimating the tail of the Dyson expansion, so for small t the above expression allows one to compute upper and lower bounds on the transition probabilities. The reader is asked to compute a specific example in Problem 67.

We come now to the main theorem in this section. Since the proof is the same in the case where $A(t)$ generates a contraction semigroup on a Banach space X, we give the proof in this more general setting. The idea of the proof is very simple and direct. For each positive integer k, we define an approximate propagator $U_k(s, t)$ on $0 \le s \le t \le 1$ by

$$U_k(t, s) = \exp\left(-(t - s)A\left(\frac{i-1}{k}\right)\right) \quad \text{if} \quad \frac{i-1}{k} \le s \le t \le \frac{i}{k} \quad (\text{where } 1 \le i \le k) \quad \text{(X.130a)}$$

and

$$U_k(t, r) = U_k(t, s)U_k(s, r) \quad \text{if} \quad 0 \le r \le s \le t \le 1 \quad \text{(X.130b)}$$

That is, $U_k(t, s)$ is defined by the constant generator $A((i-1)/k)$ for s and t in the small intervals $[(i-1)/k, i/k]$ and by the product formula when s and t are not both in the same small interval. We will show that under suitable hypotheses, $U_k(t, s)$ converges to a propagator $U(t, s)$ so that $\varphi_s(t) = U(t, s)\psi$ solves $d\varphi_s(t)/dt = -A(t)\varphi_s(t)$. To see what these hypotheses should be we compute formally

$$(U_k(t, 0) - U_n(t, 0))A(0)^{-1}\varphi = [U_n(t, s)U_k(s, 0)A(0)^{-1}\varphi]_{s=0}^{s=t}$$

$$= \int_0^t \frac{d}{ds}(U_n(t, s)U_k(s, 0)A(0)^{-1}\varphi)\, ds$$

$$= \int_0^t U_n(t, s)\left\{A\left(\frac{[ns]}{n}\right) - A\left(\frac{[ks]}{k}\right)\right\}$$

$$\times A\left(\frac{[ks]}{k}\right)^{-1} A\left(\frac{[ks]}{k}\right) U_k(s, 0)A(0)^{-1}\varphi\, ds \quad \text{(X.131)}$$

where $[r]$ always denotes the largest integer less than or equal to r. The fact that $A([ns]/n)$ can be written to the right of $U_n(t, s)$ follows by writing $U_n(t, s)$ as a product if t and s are not in the same small interval. Thus to show that the left-hand side of (X.131) is small, it suffices that $A(t)A(s)^{-1} - I$ be small when $|t - s|$ is small and that $A(t)U_k(t, 0)A(s)^{-1}$ be bounded. We thus define

$$C(t, s) = A(t)A(s)^{-1} - I$$

and state:

Theorem X.70 Let X be a Banach space and let I be an open interval in $\mathbb{R}$. For each $t \in I$, let $A(t)$ be the generator of a contraction semigroup on X so that $0 \in \rho(A(t))$ and

(a) The $A(t)$ have a common domain D (from which it follows by the closed graph theorem that $A(t)A(s)^{-1}$ is bounded).
(b) For each $\varphi \in X$, $(t - s)^{-1}C(t, s)\varphi$ is uniformly strongly continuous and uniformly bounded in s and t for $t \neq s$ lying in any fixed compact subinterval of I.
(c) For each $\varphi \in X$, $C(t)\varphi \equiv \lim_{s \uparrow t}(t - s)^{-1}C(t, s)\varphi$ exists uniformly for t in each compact subinterval and $C(t)$ is bounded and strongly continuous in t.

Then for all $s \le t$ in any compact subinterval of I and any $\varphi \in X$,

$$U(t, s)\varphi = \lim_{k \to \infty} U_k(t, s)\varphi$$

exists uniformly in s and t. Further, if $\psi \in D$, then $\varphi_s(t) \equiv U(t, s)\psi$ is in D for all t and satisfies

$$\frac{d}{dt}\varphi_s(t) = -A(t)\varphi_s(t), \qquad \varphi_s(s) = \psi$$

and $\|\varphi_s(t)\| \le \|\psi\|$ for all $t \ge s$.

We make two remarks. First, the hypothesis that $0 \in \rho(A(t))$ is usually not a strong restriction. If we can find a $z_0 \in \rho(A(t))$ for all t and if the operators $B(t) = A(t) - z_0$ satisfy the hypothesis, then $\tilde{U}(t, s) = U(t, s)e^{(s-t)z_0}$ is a propagator for $A(t)$ if $U(t, s)$ is the propagator for $B(t)$. In particular, when $A(t)$ is i times a self-adjoint operator, we can use this trick. Secondly, it is sufficient to prove the existence of the propagator for s, $t \in [0, 1]$ since we can then use the same procedure to extend to $[1, 2]$ and so forth. We begin by showing that the hypotheses imply the boundedness of $A(t)U(t, s)A(s)^{-1}$.

Lemma For s, $t \in [0, 1]$ define $W_k(t, s) = A(t)U_k(t, s)A(s)^{-1}$. Then $\|W_k(t, s)\| \le M_1$ independent of s, t, and k.

Proof Fix s, t, and k. Since $U_k(t, s)\colon D \to D$, $W_k(t, s)$ is well defined on X. Letting $\psi \in X$, we write $W_k(t, s)$ as

$$\begin{aligned}
W_k(t, s)\psi &= A(t)U_k\left(t, \frac{[kt]}{k}\right)U_k\left(\frac{[kt]}{k}, \frac{[kt]-1}{k}\right)\cdots U_k\left(\frac{[ks]+1}{k}, s\right)A(s)^{-1}\psi \\
&= A(t)A\left(\frac{[kt]}{k}\right)^{-1}U_k\left(t, \frac{[kt]}{k}\right)A\left(\frac{[kt]}{k}\right)A\left(\frac{[kt]-1}{k}\right)^{-1}\cdots \\
&\quad \times A\left(\frac{[ks]}{k}\right)^{-1}U_k\left(\frac{[ks]+1}{k}, s\right)A\left(\frac{[ks]}{k}\right)A(s)^{-1}\psi \\
&= \left(I + C\left(t, \frac{[kt]}{k}\right)\right)\left\{U_k(t, s) + \sum_{ku=[ks]+1}^{[kt]} U_k(t, u)C\left(u, u-\frac{1}{k}\right)U_k(u, s)\right. \\
&\quad + \sum_{kv=[ks]+1}^{[kt]} U_k(t, v)C\left(v, v-\frac{1}{k}\right)\sum_{ku=[ks]+1}^{[kt]} U_k(v, u) \\
&\quad \left.\times C\left(u, u-\frac{1}{k}\right)U_k(u, s) + \cdots\right\}\left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi \\
&= \left(I + C\left(t, \frac{[tk]}{k}\right)\right)\{U_k(t, s) + W_k^1(t, s) + W_k^2(t, s) + \cdots\} \\
&\quad \times \left(I + C\left(\frac{[ks]}{k}, s\right)\right)\psi
\end{aligned}$$

where

$$W_k^1(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u-\frac{1}{k}\right)U_k(u, s)$$

and

$$W_k^{m+1}(t, s) = \sum_{ku=[ks]+1}^{[kt]} U_k(t, s)C\left(u, u-\frac{1}{k}\right)W_k^m(u, s) \tag{X.132}$$

Let

$$M_2 = \sup_{t \ne s}\|(t-s)^{-1}C(t, s)\|$$

Then

$$\left\|C\left(u, u-\frac{1}{k}\right)\psi\right\| \le \frac{M_2}{k}\|\psi\|$$

so from (X.132) we have

$$\|W_k^1(t, s)\psi\| \le (t-s)M_2\|\psi\| \qquad \text{and} \qquad \|W_k^m(t, s)\psi\| \le \frac{(t-s)^m}{m!}M_2^m\|\psi\|$$

Therefore

$$\|W_k(t, s)\| \le \left(1 + \frac{M_2}{k}\right)^2\left(1 + \sum_{m=1}^{\infty}\frac{(t-s)^m}{m!}M_2^m\right)\|\psi\|$$

We have repeatedly used the fact that $\|U_k(r_1, r_2)\psi\| \le \|\psi\|$ since each $A(t)$ generates a contraction semigroup. ∎

Proof of Theorem X.70 Let $\varphi \in D$. Since $U_k(r, s)\varphi \in D$ for $r \ge s$ and

$$U_k(t, s)\varphi = e^{-(t-[kt]/k)A([kt]/k)}U_k\left(\frac{[kt]}{k}, s\right)\varphi$$

we see that $U_k(t, s)$ is strongly differentiable in t except when $t = j/k$, and letting $A(0)\varphi = \psi$,

$$\begin{aligned}
\frac{d}{dt}U_k(t, s)\varphi &= -A\left(\frac{[kt]}{k}\right)U_k(t, s)\varphi \\
&= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}A(t)U_k(t, s)A(s)^{-1}A(s)A(0)^{-1}\psi \\
&= -A\left(\frac{[kt]}{k}\right)A(t)^{-1}W_k(t, s)A(s)A(0)^{-1}\psi
\end{aligned}$$

Thus, since $\|W_k(t, s)\|$ is uniformly bounded and $C(t, s)$ is strongly continuous, we see that $dU_k(t, s)\varphi/dt$ is bounded and strongly continuous

except at $t = j/k$. A similar proof shows that the same conclusion holds for

$$\frac{d}{ds} U_k(t, s)\varphi = -U_k(t, s)A\left(\frac{[ks]}{k}\right)\varphi$$

when $s \neq j/k$. Thus if $k > n$,

$$\begin{aligned}
&(U_k(t, s) - U_n(t, s))A(0)^{-1}\psi \\
&\quad = [U_n(t, r)U_k(r, s)]_{r=s}^{r=t} A(0)^{-1}\psi \\
&\quad = \int_s^t \frac{d}{dr}\{U_n(t, r)U_k(r, s)A(0)^{-1}\psi\}\, dr \qquad \text{(X.133)} \\
&\quad = \int_s^t U_n(t, r)\left\{A\left(\frac{[rn]}{n}\right) - A\left(\frac{[rk]}{k}\right)\right\}A\left(\frac{[rn]}{n}\right)^{-1} A\left(\frac{[rn]}{n}\right)U_k(r, s)A(0)^{-1}\psi\, dr \\
&\quad = \int_s^t U_n(t, r)C\left(\frac{[rn]}{n}, \frac{[rk]}{k}\right)\left\{1 + C\left(\frac{[rn]}{n}, r\right)\right\}W_k(r, s)\{1 + C(s, 0)\}\psi\, dr
\end{aligned}$$

Since

$$\left\|C\left(\frac{[rk]}{k}, \frac{[rn]}{n}\right)\right\| \leq 2\left|\frac{[rk]}{k} - \frac{[rn]}{n}\right| \sup_{s \neq t}|t - s|^{-1}\|C(t, s)\|$$

and $U_n(t, r)$, $C([rn]/n, r)$, $C(s, 0)$, and $W_k(r, s)$ (by the lemma) are all uniformly bounded independent of r, s, t, n, and k, we see that the strong limit of $U_k(t, s)$ exists uniformly in t and s. Since $U_k(t, s)$ is uniformly bounded

$$U(t, s)\varphi \equiv \lim_{k \to \infty} U_k(t, s)\varphi$$

exists for all $\varphi \in X$ and $U(t, s)$ is a bounded-operator-valued function and is uniformly strongly jointly continuous. We remark that the integral (X.133) is really a sum of integrals over the intervals where the derivative exists.

A similar proof shows that

$$W(t, s)\varphi \equiv \lim_{k \to \infty} W_k(t, s)\varphi$$

exists boundedly and uniformly in t and s and that $W(t, s)$ is a bounded-operator-valued function which is jointly strongly continuous. Thus, if $\varphi \in D$, $U_k(t, s)\varphi \to U(t, s)\varphi$ and

$$\begin{aligned}
A(t)U_k(t, s)\varphi &= W_k(t, s)A(s)\varphi \\
&\xrightarrow[k \to \infty]{} W(t, s)A(s)\varphi
\end{aligned}$$

Since $A(t)$ is closed, this implies that $U(t, s)\varphi \in D$ and $A(t)U(t, s)\varphi = W(t, s)A(s)\varphi$. Furthermore

$$\begin{aligned}
U(t, s)\varphi - \varphi &= \lim_{k \to \infty}(U_k(t, s)\varphi - \varphi) \\
&= \lim_{k \to \infty} \int_s^t \frac{d}{dr} U_k(r, s)\varphi\, dr \\
&= \lim_{k \to \infty} -\int_s^t A\left(\frac{[rk]}{k}\right)U_k(r, s)\varphi\, dr \\
&= -\lim_{k \to \infty} \int_s^t A\left(\frac{[rk]}{k}\right)A(r)^{-1}A(r)U_k(r, s)A(s)^{-1}A(s)\varphi\, dr \\
&= -\int_s^t W(r, s)A(s)\varphi\, dr
\end{aligned}$$

Since $W(r, s)$ is strongly continuous,

$$\frac{d}{dt} U(t, s)\varphi = -W(t, s)A(s)\varphi = -A(t)U(t, s)\varphi$$

which concludes the proof of Theorem X.70. ∎

Example 2 We can easily apply this result to the heat equation with time-dependent sources and sinks proportional to the temperature. Let $q(x, t)$ be a bounded real-valued continuously differentiable function on $\mathbb{R}^{n+1}$ so that $\partial q(x, t)/\partial t$ is bounded. Let M be the bound of q and set

$$A(t) = -\Delta + q(x, t) + (M + 1)$$

on $C_\infty(\mathbb{R}^n)$. From Examples 3 and 4 in Section X.8 we know that $A(t)$ is the generator of a contraction semigroup on $C_\infty(\mathbb{R}^n)$ and that $D(A(t)) = D(-\Delta)$ for all t. The reader can easily check (Problem 68) that the hypotheses on $q + M + 1$ imply that the conditions of Theorem X.70 are satisfied. Thus for each $\psi \in D(-\Delta)$ there is a function $\tilde{\varphi}(x, t)$ so that for each t, $\tilde{\varphi}(x, t) \in D(-\Delta)$ and

$$\begin{aligned}
\frac{d}{dt}\tilde{\varphi}(x, t) &= \Delta\tilde{\varphi}(x, t) - q(x, t)\tilde{\varphi}(x, t) - (M + 1)\tilde{\varphi}(x, t) \\
\tilde{\varphi}(x, 0) &= \psi(x)
\end{aligned}$$

If we now define $\varphi(x, t) = e^{(M+1)t}\tilde{\varphi}(x, t)$, then $\varphi(x, t)$ satisfies

$$\begin{aligned}
\frac{d}{dt}\varphi(x, t) &= \Delta\varphi(x, t) - q(x, t)\varphi(x, t) \\
\varphi(x, 0) &= \psi(x)
\end{aligned}$$

Notice that $U_k(t, s)$ is positivity preserving for each k since it is the product of positivity-preserving transformations (see Example 4 in Section X.8). Thus $U(t, s)$ is positivity preserving since it is the strong limit of the $U_k(t, s)$. Therefore, given any nonnegative initial data $\psi \in C_\infty(\mathbb{R})$, the solution $\varphi(x, t) = e^{(M+1)t}U(t, s)\psi$ will remain nonnegative corresponding to our intuition about heat flow.

Finally, we apply Theorem X.70 to the quantum mechanical case.

Theorem X.71 Let $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and suppose that $t \to V_1(t)$ and $t \to V_2(t)$ are continuously differentiable $L^2(\mathbb{R}^3)$-valued and $L^\infty(\mathbb{R}^3)$-valued functions respectively. Let $V(t) = V_1(t) + V_2(t)$ and set $H(t) = H_0 + V(t)$. Then there is a unitary propagator $U(t, s)$ on $L^2(\mathbb{R}^3)$ so that for each $\psi \in D(H_0)$, $\varphi_s(t) = U(t, s)\psi$ is strongly differentiable and satisfies

$$\frac{d}{dt}\varphi_s(t) = -iH(t)\varphi_s(t), \qquad \varphi_s(s) = \psi \tag{X.134}$$

Proof We will construct a unitary propagator for each finite interval $[-T, T]$. By Theorem X.15, $H_0 + V(t)$ is self-adjoint on $D(-\Delta)$ for each t. Further, since $V_1(t)$ and $V_2(t)$ are uniformly bounded in L^2 and L^∞ norm respectively, we can find a constant $D \geq 0$ so that $H_0 + V(t) + D \geq \frac{1}{2}$ for all $t \in [-T, T]$. Thus $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ generate contraction semigroups for each t and $(\pm i(H_0 + V(t) + D))^{-1}$ exists for $t \in [-T, T]$. Further, the hypotheses on $t \to V_1(t)$ and $t \to V_2(t)$ imply that $i(H_0 + V(t) + D)$ and $-i(H_0 + V(t) + D)$ satisfy the hypotheses (b) and (c) of Theorem X.70. Let $U^+(t, s)$ and $U^-(t, s)$ be the corresponding propagators. Since U_k^+ and U_k^- are unitary for each k, U^+ and U^- are unitary. Now define

$$\tilde{U}(t, s) = \begin{cases} U^+(t, s), & s \leq t \\ U^-(s, t), & t \leq s \end{cases}$$

and

$$U(t, s) = e^{iD(t-s)}\tilde{U}(t, s) \quad \blacksquare$$

We conclude this section with a brief outline of a method due to J. Howland for turning time-dependent problems into time-independent problems. In classical mechanics, Hamilton's equations for a system with Hamiltonian function $H(p_1, \ldots, p_n, q_1, \ldots, q_n, t)$ are

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{dt} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \tag{X.135}$$

If H depends on t, energy is not conserved by such a system, but we can set up a corresponding energy conserving system by introducing t as a coordinate and the energy E of the external source as its conjugate momentum. The new Hamiltonian is

$$h(\mathbf{p}, \mathbf{q}, t, E) = E + H(\mathbf{p}, \mathbf{q}, t)$$

so if we denote by σ the new time variable, Hamilton's equations read

$$\begin{aligned} &\frac{dq_i}{d\sigma} = \frac{\partial H}{\partial p_i}, \qquad -\frac{dp_i}{d\sigma} = \frac{\partial H}{\partial q_i}, \qquad i = 1, \ldots, n \\ &\frac{dt}{d\sigma} = \frac{\partial h}{\partial E} = 1, \qquad -\frac{dE}{d\sigma} = \frac{\partial H}{\partial t} \end{aligned} \tag{X.136}$$

This set of equations is equivalent to (X.135).

We can reformulate the quantum-mechanical problem similarly. Let $H(t)$ be a family of self-adjoint operators on a Hilbert space $\mathscr{H}$ and set $\mathscr{H}_1 = L^2(\mathbb{R}; \mathscr{H})$, the Hilbert space of strongly measurable $\mathscr{H}$-valued functions $f(\cdot)$ on $\mathbb{R}$ such that $\int_{-\infty}^{\infty} \|f(t)\|_{\mathscr{H}}^2 \, dt < \infty$. If we now define h on $\mathscr{H}_1$ by

$$(hf)(t) = -i\frac{d}{dt}f(t) + H(t)f(t)$$

there should be (according to the classical analogy) a correspondence between the solutions of

$$\frac{d}{d\sigma}\varphi(\sigma) = -ih\varphi(\sigma)$$

on $\mathscr{H}_1$ and the solutions of the time-dependent problem (X.134) on $\mathscr{H}$. Suppose that $U(t, s)$ is a unitary propagator on $\mathscr{H}$. Then

$$(\hat{U}(\sigma)f)(t) \equiv U(t, t - \sigma)f(t - \sigma) \tag{X.137}$$

is a strongly continuous unitary group on $\mathscr{H}_1$ (Problem 69). Notice that this means that if T_σ is the group on $\mathscr{H}_1$ which acts by $(T_\sigma f)(t) = f(t + \sigma)$, then $\hat{U}(\sigma)T_\sigma$ acts on $\mathscr{H}_1$ by multiplication by an operator-valued function. Conversely, one can prove that to each strongly continuous unitary group $\hat{U}(\sigma)$ on $\mathscr{H}$, so that $\hat{U}(\sigma)T_\sigma$ is multiplication by an operator-valued function, there corresponds a unique unitary propagator $U(t, s)$ on $\mathscr{H}$ so that (X.137) holds. Thus, we have a correspondence between unitary propagators on $\mathscr{H}$ and certain strongly continuous one-parameter unitary groups on $\mathscr{H}_1$. Notice that $\hat{U}(\sigma)$ will always be strongly differentiable on a dense set in $\mathscr{H}_1$ by Stone's theorem, but that $U(t, s)$ need not be strongly

differentiable on $\mathscr{H}$. Thus, we have a method of proving the existence of propagators in situations where we might not expect strong differentiability, i.e., situations where we cannot use Theorem X.70. This propagator formally solves

$$\frac{d}{dt}U(t,s)\psi = -iH(t)U(t,s)\psi$$

Example 3 We will consider again the case $H(t) = H_0 + V(t)$ where H_0 is a self-adjoint operator on $\mathscr{H}$ and $t \to V(t)$ is a strongly continuous map from $\mathbb{R}$ to the bounded operators on $\mathscr{H}$. To make things easier, we will assume that $\|V(t)\|$ is uniformly bounded on all of $\mathbb{R}$. As before we let $\tilde{V}(t) = e^{iH_0t}V(t)e^{-iH_0t}$. Let $\hat{\tilde{V}}$ be the operator on $L^2(\mathbb{R};\mathscr{H})$ which acts by $(\hat{\tilde{V}}f)(t) = \tilde{V}(t)f(t)$ and let $C_0^1(\mathbb{R};\mathscr{H})$ denote the continuously differentiable $\mathscr{H}$-valued functions on $\mathbb{R}$ with compact support. Then it is not hard to check that $i^{-1}\,d/dt$ is essentially self-adjoint on $C_0^1(\mathbb{R};\mathscr{H})$. Since $\hat{\tilde{V}}$ is a bounded operator, $i^{-1}\,d/dt + \hat{\tilde{V}}$ is also essentially self-adjoint on $C_0^1(\mathbb{R};\mathscr{H})$ and it is possible to show that $\exp(-i\sigma(i^{-1}\,d/dt + \hat{\tilde{V}}))T_\sigma$ operates by multiplication by an operator-valued function. Thus by the correspondence theorem mentioned above, there is a strongly continuous propagator $\tilde{U}(t,s)$ on $\mathscr{H}$ so that

$$\left(\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)f\right)(t) = \tilde{U}(t, t-\sigma)f(t-\sigma)$$

One can easily check that this $\tilde{U}$ is just the propagator arising from applying the Dyson expansion to $t \to \tilde{V}(t)$. Now, let $\hat{W}$ act on $L^2(\mathbb{R};\mathscr{H})$ by $(\hat{W}f)(t) = e^{-iH_0t}f(t)$. Then $\hat{W}$ is unitary so

$$\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}$$

is again a strongly continuous unitary group on $L^2(\mathbb{R};\mathscr{H})$ and clearly

$$\left(\hat{W}\exp\left(-i\sigma\left(\frac{1}{i}\frac{d}{dt} + \hat{\tilde{V}}\right)\right)\hat{W}^{-1}f\right)(t) = e^{-itH_0}\tilde{U}(t, t-\sigma)e^{i(t-\sigma)H_0}f(t-\sigma)$$

So $U(t,s) = e^{-itH_0}\tilde{U}(t,s)e^{isH_0}$ is the propagator on $\mathscr{H}$ which formally solves

$$\frac{d}{dt}U(t,s) = -i(H_0 + V(t))U(t,s)$$

since the generator of $\hat{W}\exp(-i\sigma(i^{-1}\,d/dt + \hat{\tilde{V}}))\hat{W}^{-1}$ is $i^{-1}d/dt + H_0 + \hat{\tilde{V}}$.

X.13 Classical nonlinear wave equations

A thorough discussion of nonlinear partial differential equations is outside the scope of this book. However, we want to describe some of the functional analytic techniques which are useful in studying these classical problems. We will use the nonlinear Klein–Gordon equation as a motivating example. Suppose that $m, \lambda > 0$, and let two functions f and g on $\mathbb{R}^3$ be given. The problem is to prove the existence and study the behavior of a function $u(x,t)$ satisfying

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} - \Delta u + m^2 u &= -\lambda|u|^2u\\ u(x,0) &= f(x)\\ \frac{\partial u}{\partial t}(x,0) &= g(x)\end{aligned} \tag{X.138}$$

In this section we treat the existence, uniqueness, and smoothness of solutions of (X.138). In Section XII.13, we develop a scattering theory for (X.138). We are treating the Klein–Gordon problem for complex-valued functions u. If the initial data f and g are real valued, then u will be real valued for all t (Problem 71) and thus satisfies

$$u_{tt} - \Delta u + m^2u = -\lambda u^3 \tag{X.139}$$

This equation is the classical analogue of the φ^4 quantum field theory equation discussed in Section X.7.

Classical field theories like those described by (X.139) are formally in the form of Hamiltonian systems. If we let

$$H(u,v) = \frac{1}{2}\int\left(v(x)^2 + (\nabla u(x))^2 + m^2u(x)^2 + \frac{\lambda}{2}u(x)^4\right)d^3x$$

then (X.139) is formally equivalent to

$$u_t(x) = \frac{\delta H}{\delta v(x)} = v(x)$$

$$v_t(x) = -\frac{\delta H}{\delta u(x)} = (\Delta - m^2)u(x) - \lambda(u(x))^3$$

where we have integrated by parts to obtain

$$\int(\nabla u(x))^2\,d^3x = -\int u(x)\,\Delta u(x)\,d^3x$$

This suggests that, as in classical Hamiltonian systems with a finite number of degrees of freedom, the total energy should be conserved. That is, if u is a sufficiently smooth solution of (X.139) which falls off fast enough at infinity to justify integrations by parts and differentiation under the integral sign, then $H(u, u_t)$ should be time independent. Such a conservation law will be crucial for the *global* existence theory of (X.138) and (X.139) and will distinguish between the cases $\lambda > 0$ and $\lambda < 0$. If $\lambda > 0$, then as time develops both u and ∇u are prevented from getting large, since neither can get large without $H(u, u_t)$ getting large. On the other hand if $\lambda < 0$, then both u and ∇u can get large in such a way that their contributions to $H(u, u_t)$ cancel. Thus, one expects global solutions to exist if $\lambda > 0$ and we prove this by exploiting conservation of energy. If $\lambda < 0$, we expect that for some initial data global solutions will not exist. This situation is analogous to the situation with the ordinary differential equation

$$m\ddot{q}(t) = \lambda q^3(t)$$

Since the energy $\frac{1}{2}m\dot{q}^2 + \frac{1}{4}\lambda q^4$ is conserved, the solution cannot get to infinity in finite time if $\lambda > 0$, so global solutions exist; but if $\lambda < 0$, the solution does get to infinity in finite time.

Since the techniques which we have developed in this chapter so far apply to differential equations of first order in t, we rewrite (X.138) as a first-order system:

$$\frac{\partial v}{\partial t} - \Delta u + m^2 u = -\lambda |u|^2 u$$

$$\frac{\partial u}{\partial t} = v$$

$$u(x, 0) = f(x)$$

$$v(x, 0) = g(x)$$

or

$$\dot{\varphi}(t) - \begin{pmatrix} 0 & I \\ \Delta - m^2 & 0 \end{pmatrix} \varphi(t) = J(\varphi(t))$$

$$\varphi(x, 0) = \begin{pmatrix} f(x) \\ g(x) \end{pmatrix} \tag{X.140}$$

where

$$\varphi = \begin{pmatrix} u \\ v \end{pmatrix} \quad \text{and} \quad J(\varphi) = \begin{pmatrix} 0 \\ -\lambda |u|^2 u \end{pmatrix}$$

From now on we write column vectors as row vectors. Our plan is to formulate (X.140) as a Hilbert space problem and then prove a general Hilbert space theorem guaranteeing existence and uniqueness. Let $B \geq mI$ be the positive square root of a strictly positive self-adjoint operator B^2 on a Hilbert space $\mathscr{H}$. (In our case $\mathscr{H} = L^2(\mathbb{R}^3)$ and $B^2 = -\Delta + m^2$.) Since B^2 is closed, the domain of B, $D(B)$, is a Hilbert space under the inner product (Bu, Bu). We will denote by $\mathscr{H}_B$ the direct sum $\mathscr{H}_B \equiv D(B) \oplus \mathscr{H}$ with the inner product

$$(\langle u, v\rangle, \langle u, v\rangle)_B \equiv (Bu, Bu) + (v, v)$$

Let

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix} \tag{X.141}$$

Then it is easy to check that A is a symmetric operator on $\mathscr{H}_B$ with domain $D \equiv D(B^2) \oplus D(B)$ and that A is closed since B and B^2 are closed. Now, defining $\cos(tB)$ and $\sin(tB)$ by the functional calculus, we set

$$W(t) = \begin{pmatrix} \cos(tB) & B^{-1}\sin(tB) \\ -B\sin(tB) & \cos(tB) \end{pmatrix}$$

Then $W(t)$ is a strongly continuous unitary group on $\mathscr{H}_B$. Furthermore, if $u \in D$, the strong derivative of $W(t)u$ exists at zero and equals $-iA$ and $W(t)$ takes D into itself. Thus, by Theorem VIII.11, the generator of $W(t)$ is essentially self-adjoint on D. Since A is closed, A is self-adjoint on D and is the infinitesimal generator of $W(t)$. We summarize in a proposition.

Proposition Let B be a strictly positive self-adjoint operator on a Hilbert space $\mathscr{H}$. Then $W(t)$ is a strongly continuous one-parameter unitary group on $\mathscr{H}_B$ whose infinitesimal generator

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}$$

is self-adjoint on $D = D(B^2) \oplus D(B)$.

We can now formulate an abstract version of (X.140). Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ (no longer necessarily of the form (X.141)) and suppose that J is a nonlinear mapping from $D(A)$ to $\mathscr{H}$. The problem is to find conditions on J guaranteeing that for each $\varphi_0 \in D(A)$, there is a unique $\mathscr{H}$-valued function $\varphi(t)$ on $[0, \infty)$ satisfying

$$\frac{d\varphi}{dt} = -iA\varphi + J(\varphi)$$

$$\varphi(0) = \varphi_0 \tag{X.142}$$

The technique of proof is to reformulate (X.142) as an integral equation

$$\varphi(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds \tag{X.143}$$

and prove the existence of unique local solutions of (X.143) by the contraction mapping principle. Our conditions on J will be strong enough to guarantee that any solution of (X.143) is automatically a solution of (X.142). It is possible to weaken the conditions on J so that one obtains solutions of (X.143) but not of (X.142) because the solution is not necessarily strongly differentiable.

Theorem X.72 (local existence) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a mapping from $D(A)$ to $D(A)$ which satisfies:

(H_0) $\quad \|J(\varphi)\| \le C(\|\varphi\|)\|\varphi\|$

(H_1) $\quad \|AJ(\varphi)\| \le C(\|\varphi\|, \|A\varphi\|)\|A\varphi\|$

(H_0^L) $\quad \|J(\varphi) - J(\psi)\| \le C(\|\varphi\|, \|\psi\|)\|\varphi - \psi\|$

(H_1^L) $\quad \|A(J(\varphi) - J(\psi))\| \le C(\|\varphi\|, \|A\varphi\|, \|\psi\|, \|A\psi\|)\|A\varphi - A\psi\|$

for all $\varphi, \psi \in D(A)$ where each constant C is a monotone increasing (everywhere finite) function of the norms indicated. Then, for each $\varphi_0 \in D(A)$ there is a $T > 0$ so that (X.142) has a unique continuously differentiable solution for $t \in [0, T)$. For each set of the form $\{\varphi \mid \|\varphi\| \le a, \|A\varphi\| \le b\}$, T can be chosen uniformly for all φ_0 in the set.

Proof Let X_T be the set of $D(A)$-valued functions on $[0, T)$ for which $\varphi(t)$ and $A\varphi(t)$ are continuous and

$$\|\varphi(\cdot)\|_T \equiv \sup_{t \in [0, T)} \|\varphi(t)\| + \sup_{t \in [0, T)} \|A\varphi(t)\| < \infty$$

Since A is a closed operator, X_T with the norm $\|\varphi(\cdot)\|_T$ is a Banach space. Choose some fixed $\varepsilon > 0$. Let $\varphi_0 \in D(A)$ be given and let $X_{T, \varepsilon, \varphi_0}$ consist of those $\varphi(\cdot)$ in X_T with $\varphi(0) = \varphi_0$ and $\|\varphi(\cdot) - e^{-iAt}\varphi_0\|_T \le \varepsilon$. We will show that the map

$$(S\varphi)(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)} J(\varphi(s))\, ds \tag{X.144}$$

is a contraction on $X_{T, \varepsilon, \varphi_0}$ if T is small enough. We denote by C_ε any of the constants in the hypotheses with arguments $\|\varphi_0\| + \varepsilon$ and $\|A\varphi_0\| + \varepsilon$. Suppose that $\varphi(\cdot) \in X_{T, \varepsilon, \varphi_0}$; then

$$\begin{aligned}
&\|e^{-iA(t-(s+h))} J(\varphi(s+h)) - e^{-iA(t-s)} J(\varphi(s))\| \\
&\quad \le \|J(\varphi(s+h)) - J(\varphi(s))\| + \|(e^{-iAh} - I)J(\varphi(s))\| \\
&\quad \le C_\varepsilon \|\varphi(s+h) - \varphi(s)\| + \|(e^{-iAh} - I)J(\varphi(s))\|
\end{aligned}$$

so $e^{-iA(t-s)}J(\varphi(s))$ is a continuous $\mathscr{H}$-valued function of s. A similar proof shows that $Ae^{-iA(t-s)}J(\varphi(s))$ is also continuous. Thus, the right-hand side of (X.144) can be defined using the Riemann integral, and if

$$\eta_n(t) \equiv \sum_{m=1}^{n} \frac{1}{n} e^{-i(t-(m/n)t)A} J\left(\varphi\left(\frac{m}{n}t\right)\right)$$

and

$$\eta(t) \equiv \int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds$$

then $\eta_n(t) \to \eta(t)$ as $n \to \infty$. Now, by the hypotheses on J, each $\eta_n(t) \in D(A)$, so

$$\begin{aligned}
A\eta_n(t) &= \sum_{m=1}^{n} \frac{1}{n} e^{-i(t-(m/n)t)A} AJ\left(\varphi\left(\frac{m}{n}t\right)\right) \\
&\to \int_0^t e^{-i(t-s)A} AJ(\varphi(s))\, ds
\end{aligned}$$

Therefore, $\eta(t) \in D(A)$ and

$$A\int_0^t e^{-i(t-s)A} J(\varphi(s))\, ds = \int_0^t e^{-i(t-s)A} AJ(\varphi(s))\, ds \tag{X.145}$$

Further,

$$\begin{aligned}
\|A\eta(t+h) - A\eta(t)\| &\le \left\| \int_t^{t+h} e^{-iA(t-s)} e^{-iAh} AJ(\varphi(s))\, ds \right\| \\
&\quad + \left\| \int_0^t (e^{-ihA} - I) e^{-iA(t-s)} AJ(\varphi(s))\, ds \right\| \\
&\le hC_\varepsilon \|\varphi\|_T + \int_0^t \|(e^{-ihA} - I)AJ(\varphi(s))\|\, ds
\end{aligned}$$

The integrand in the second term converges to zero as $h \to 0$ for each s and by the hypotheses on J, the integrand is uniformly bounded. Thus, by the dominated convergence theorem the right-hand side converges to zero as $h \to 0$, so $A\eta(t)$ is continuous and similarly, $\eta(t)$ is continuous. Further, exactly the same kind of estimates as above show that for any $\varphi(\cdot)$, $\psi(\cdot) \in X_{T, \varepsilon, \varphi_0}$, we have

$$\|(S\varphi)(t) - e^{-iAt}\varphi_0\| \le C_\varepsilon T \sup_{t \in [0, T)} \|\varphi(t)\|$$

$$\|A(S\varphi)(t) - Ae^{-iAt}\varphi_0\| \le C_\varepsilon T \sup_{t \in [0, T)} \|A\varphi(t)\|$$

$$\|(S\varphi)(t) - (S\psi)(t)\| \le C_\varepsilon T \sup_{t \in [0, T)} \|\varphi(t) - \psi(t)\|$$

$$\|A[(S\varphi)(t) - (S\psi)(t)]\| \le C_\varepsilon T \sup_{t \in [0, T)} \|A\varphi(t) - A\psi(t)\|$$

Thus, for T small enough, S is a contraction on $X_{T,\varepsilon,\varphi_0}$ so, by Theorem V.18, S has a unique fixed point $\varphi(\cdot)$ in $X_{T,\varepsilon,\varphi_0}$ which satisfies (X.143).

Now, suppose that $\tilde{\varphi}$ is a continuously differentiable $D(A)$-valued solution of (X.142) on the interval $[0, \tilde{T})$ with $\tilde{\varphi}(0) = \varphi_0$. By the differential equation, $A\tilde{\varphi}(t)$ is continuous, so $\tilde{\varphi}(t) \in X_{T,\varepsilon,\varphi_0}$ for t in some interval $[0, T_0)$. Since $\tilde{\varphi}$ obeys (X.143), $\varphi(t) = \tilde{\varphi}(t)$ for $t < T_0$. Let T_1 be the sup of such T_0. Then since $X_{T,\varepsilon,\varphi_0}$ is closed, $\tilde{\varphi}(T_1) \in X_{T,\varepsilon,\varphi_0}$. Now, if $T_1 < T$, then since $\tilde{\varphi}(T_1) = \varphi(T_1)$ the same argument as above shows that $\tilde{\varphi}(t) = \varphi(t)$ for some small interval of $T_1 \le t < T_2 < T$ which contradicts the maximality of T_1. Thus $T_1 \ge T$, so $\tilde{\varphi}(t) = \varphi(t)$ for $t \in [0, T)$. That is, any strong solution of (X.142) on $[0, T)$ equals $\varphi(t)$.

To prove the strong differentiability of $\varphi(t)$ we write

$$\frac{\varphi(t+h) - \varphi(t)}{h} = \left(\frac{e^{-iAh} - I}{h}\right) e^{-iAt}\varphi_0 + \frac{1}{h}\int_t^{t+h} e^{-iA(t-s)} e^{-ihA} J(\varphi(s))\, ds + \int_0^t e^{-iA(t-s)} \left(\frac{e^{-ihA} - I}{h}\right) J(\varphi(s))\, ds \tag{X.146}$$

Since $\varphi_0 \in D(A)$ the first term converges to $-iAe^{-iAt}\varphi_0$ as $h \to 0$ and since the integrand of the second term is continuous, it converges to $J(\varphi(t))$. The integrand of the third term converges to $e^{-iA(t-s)}(-iAJ(\varphi(s)))$ for each s and

$$\left\| \frac{e^{-ihA} - I}{h} J(\varphi(s)) \right\| \le \|AJ(\varphi(s))\| \le C\|A\varphi_0\| + \varepsilon$$

so the integrand is uniformly bounded. Thus, by the dominated convergence theorem the third term converges as $h \to 0$ to $\int_0^t e^{-iA(t-s)}\,(-iAJ(\varphi(s)))\, ds$ which by (X.145) equals $-iA\int_0^t e^{-iA(t-s)} J(\varphi(s))\, ds$. Therefore $\varphi(t)$ is strongly differentiable for $t \in [0, T)$ and satisfies (X.142). ∎

Uniqueness in the above theorem actually holds in a considerably stronger sense (Problem 72). We remark that the hypotheses H_j in the above and the following theorem follow from the hypotheses H_j^L. We state them separately for easy comparison with the hypotheses of Theorem X.74.

Theorem X.73 (local smoothness)

(a) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a mapping which takes $D(A^j)$ into $D(A^j)$ for all $1 \le j \le n$ and which satisfies (for $j = 0, 1, \ldots, n$)

(H_j) $\quad \|A^j J(\varphi)\| \le C(\|\varphi\|, \ldots, \|A^j\varphi\|)\|A^j\varphi\|$

(H_j^L) $\quad \|A^j(J(\varphi) - J(\psi))\| \le C(\|\varphi\|, \|\psi\|, \ldots, \|A^j\varphi\|, \|A^j\psi\|)\|A^j\varphi - A^j\psi\|$

for all $\varphi, \psi \in D(A^j)$ where each constant C is a monotone increasing (everywhere finite) function of all its variables. Then for each $\varphi_0 \in D(A^n)$, $n \ge 1$, there is a T_n so that (X.142) has a unique solution $\varphi(t)$ for $t \in [0, T_n)$ with $\varphi(t) \in D(A^n)$ for all $t \in [0, T_n)$. For each set of the form $\{\varphi \mid \|A^j\varphi\| \le a_j, j = 0, \ldots, n\}$, T can be chosen uniformly for φ_0 in the set.

(b) In addition to the hypotheses in (a) assume that for each $j < n$, J has the following property: If a solution φ is j times strongly continuously differentiable with $\varphi^{(k)}(t) \in D(A^{n-k})$ and $A^{n-k}\varphi^{(k)}(t)$ is continuous for all $k \le j$, then $J(\varphi(t))$ is j times differentiable, $d^jJ(\varphi(t))/dt^j \in D(A^{n-j-1})$, and $A^{n-j-1}\, d^jJ(\varphi(t))/dt^j$ is continuous. Then the solution given in part (a) is n times strongly differentiable in t and $d^j\varphi(t)/dt^j \in D(A^{n-j})$.

Proof The proof of part (a) is essentially the same as the proof of Theorem X.72 except that we take $X^{(n)}_{T_n,\varepsilon,\varphi_0}$ to be the set of functions $\varphi(\cdot)$ on $[0, T_n)$ so that $\varphi(t), \ldots, A^n\varphi(t)$ are strongly continuous and

$$\sum_{j=0}^{n} \sup_{t \in [0,T)} \|A^j\varphi(t) - e^{-iAt}A^j\varphi_0\| \le \varepsilon$$

Then one proves that S is a contraction as before.

Part (b) is proven by induction. We know from part (a) that $\varphi(t)$ is strongly continuously differentiable and $\varphi'(t) = -iA\varphi(t) + J(\varphi(t))$. By the same arguments as in Theorem X.72,

$$A\varphi(t) = Ae^{-iAt}\varphi_0 + A\int_0^t e^{-iA(t-s)}J(\varphi(s))\, ds = e^{-iAt}A\varphi_0 + \int_0^t e^{-iA(t-s)}AJ(\varphi(s))\, ds$$

and from this it follows (using another argument in Theorem X.72; see (X.146)) that $A\varphi(t)$ is strongly continuously differentiable. Therefore by the hypotheses on J, $J(\varphi(t))$ is strongly continuously differentiable, $dJ(\varphi(t))/dt \in D(A^{n-2})$, and $A^{n-2}\, dJ(\varphi(t))/dt$ is continuous. Thus, $\varphi'(t)$ is strongly differentiable,

$$\varphi''(t) = -A\varphi'(t) + \frac{d}{dt}J(\varphi(t)) = (-iA)^2\varphi(t) - iAJ(\varphi(t)) + \frac{d}{dt}J(\varphi(t))$$

$\varphi''(t) \in D(A^{n-2})$, and $A^{n-2}\varphi''(t)$ is continuous. We now repeat the argument again ($dJ(\varphi(t))/dt$ is differentiable by hypothesis since we now know that $\varphi(t)$ is twice continuously differentiable) to conclude that $\varphi(t)$ is three times strongly differentiable and so forth. ∎

Notice that the solution $\varphi(t)$ guaranteed by Theorem X.73 will generally exist on a smaller interval than the solution in Theorem X.72 since $T_n \leq T$. But by uniqueness these solutions must coincide on $[0, T_n)$. We now come to the question of whether the solution exists for all $t \geq 0$. In general this will depend on detailed properties of the nonlinear terms and not just estimates; at the end of the section we give an example where global existence does not hold. Below, we prove that if $\|\varphi(t)\|$ is a priori bounded and if we have slightly stronger estimates, then global solutions exist. Later, we will see that the conserved energy for the nonlinear Klein–Gordon equation is $\frac{1}{2}\|\varphi(t)\|^2 + \frac{1}{4}\lambda \int |u(t, x)|^4 \, d^3x$ so that $\|\varphi(t)\|$ is a priori bounded.

Lemma 1 Let A and J satisfy the hypotheses of part (a) of Theorem X.73 except that the hypotheses (H_j) are replaced by the slightly strongly hypotheses:

$$(H'_j) \qquad \|A^j J(\varphi)\| \leq C(\|\varphi\|, \ldots, \|A^{j-1}\varphi\|)\|A^j\varphi\|$$

for $1 \leq j \leq n$ (i.e., the constant does not depend on $\|A^j\varphi\|$). Let $[0, T_n)$ be a finite interval on which a solution φ of (X.142) exists with $A^j\varphi(t)$ strongly continuous on $[0, T_n)$ for each $0 \leq j \leq n$. Then, if $\|\varphi(t)\|$ is bounded on $[0, T_n)$ so is $\|A^j\varphi(t)\|$ for each $0 < j \leq n$.

Proof Since $\varphi(t)$ satisfies the differential equation on $[0, T_n)$ we have for $t \in [0, T_n)$:

$$\varphi(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\, ds$$

As before we can take A inside the integral to conclude that

$$A\varphi(t) = e^{-iAt}A\varphi_0 + \int_0^t e^{-iA(t-s)}AJ(\varphi(s))\, ds$$

so,

$$\|A\varphi(t)\| \leq \|A\varphi_0\| + \int_0^t C(\|\varphi(s)\|)\|A\varphi(s)\|\, ds$$

By hypothesis, $\|\varphi(s)\|$ is bounded on $[0, T_n)$ so there is a constant K_1 so that

$$\|A\varphi(t)\| \leq \|A\varphi_0\| + K_1 \int_0^t \|A\varphi(s)\|\, ds$$

for all $t \in [0, T_n)$. Thus by iteration we conclude that

$$\|A\varphi(t)\| \leq \|A\varphi_0\| e^{K_1 t}$$

for all $t \in [0, T_n)$ so $\|A\varphi(t)\|$ is bounded on $[0, T_n)$. Now that we know that $\|\varphi(t)\|$ and $\|A\varphi(t)\|$ are bounded, we can use (H'_2) and the same argument to conclude that $\|A^2\varphi(t)\|$ is bounded and so forth. ∎

Let $\overline{T}_n$ be the sup of the numbers T_n so that a solution $\varphi(t)$ of (X.142) exists on $[0, T_n)$ with $A^j\psi(t)$ continuous for each $j = 0, 1, \ldots, n$. By local uniqueness, each of these solutions coincide wherever their intervals of existence overlap, so the solution given by part (a) of Theorem X.73 may be extended to $[0, \overline{T}_n)$ which is called the **A^n-maximal interval** of existence of the solution.

Theorem X.74 (global existence and smoothness) Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and n a positive integer. Let J be a mapping which takes $D(A^j)$ into $D(A^j)$ for all $1 \leq j \leq n$ and which satisfies (for all $0 \leq j \leq n$)

$$(H_0) \qquad \|J(\varphi)\| \leq C(\|\varphi\|)\|\varphi\|$$

$$(H'_j) \qquad \|A^j J(\varphi)\| \leq C(\|\varphi\|, \ldots, \|A^{j-1}\varphi\|)\|A^j\varphi\|, \qquad j = 1, \ldots, n$$

$$(H^L_j) \qquad \|A^j(J(\varphi) - J(\psi))\| \leq C(\|\varphi\|, \|\psi\|, \ldots, \|A^j\varphi\|, \|A^j\psi\|)\|A^j\varphi - A^j\psi\|, \qquad j = 0, \ldots, n$$

for all $\varphi, \psi \in D(A^j)$ where each constant C is a monotone increasing (everywhere finite) function of all its variables. Let $\varphi_0 \in D(A^n)$ and suppose that on any finite interval of existence the solution $\varphi(t)$ guaranteed by part (a) of Theorem X.73 has the property that $\|\varphi(t)\|$ is bounded from above. Then there is a strongly differentiable $D(A^n)$-valued function $\varphi(t)$ on $[0, \infty)$ that satisfies

$$\begin{aligned} \varphi'(t) &= -iA\varphi(t) + J(\varphi(t)) \\ \varphi(0) &= \varphi_0 \end{aligned} \tag{X.142}$$

Further, if J satisfies the hypotheses of part (b) of Theorem X.73, then $\varphi(t)$ is n-times strongly differentiable and $d^j\varphi(t)/dt^j \in D(A^{n-j})$.

Proof Let $[0, \overline{T}_n)$ be the A^n-maximal interval of existence of the solution $\varphi(t)$ and suppose $\overline{T}_n < \infty$. By hypothesis, we know that $\|\varphi(t)\|$ is bounded on $[0, \overline{T}_n)$. This implies by Lemma 1 that $\|A^j\varphi(t)\|$ is bounded on $[0, \overline{T}_n)$ for all $0 \leq j \leq n$. Now, the length of the interval T_n over which one can use the contraction mapping principle depends only on the constants $C(\|\varphi_0\| + \varepsilon, \ldots, \|A^n\varphi_0\| + \varepsilon)$. Since they are bounded on $[0, \overline{T}_n)$, we can extend the solution $\varphi(t)$ across $\overline{T}_n$ if we choose as initial point a t_0 close enough to $\overline{T}_n$. Since this violates the maximality of $\overline{T}_n$, we conclude that $\overline{T}_n = \infty$. The rest of the statements of the theorem follow immediately from Theorem X.73. ∎

Corollary Let A and J satisfy the hypotheses of the above theorem for each $n = 0, 1, \ldots$ and suppose that J satisfies the hypotheses of part (b) of Theorem X.73. Then for each $\varphi_0 \in \bigcap_{j=1}^{\infty} D(A^j)$, (X.142) has a unique solution $\varphi(t)$ so that $\varphi(t)$ is infinitely often strongly differentiable and each derivative is in $\bigcap_{j=1}^{\infty} D(A^j)$.

We make several remarks. First, since e^{itA} is a group and all our estimates are independent of the sign of t, Theorem X.74 shows the existence of a solution for negative t as long as $\|\varphi(t)\|$ is a priori bounded on finite negative intervals also. Suppose that we have the hypothesis

$$(\mathscr{H}_0^{\mathrm{L}}) \qquad \|J(\varphi) - J(\psi)\| \leq C(\|\varphi\|, \|\psi\|)\|\varphi - \psi\| \qquad \varphi, \psi \in \mathscr{H}$$

and the a priori boundedness condition of Theorem X.47. Then by the ideas above, we can construct global solutions of the integral equation (X.143). Let M_t be the mapping

$$M_t : \varphi(0) \to \varphi(t)$$

where $\varphi(t)$ is the solution of (X.143). Then $\{M_t\}_{t \in (-\infty, \infty)}$ is a one-parameter group of everywhere defined nonlinear mappings on $\mathscr{H}$. M_t is strongly continuous since $\|\varphi(t) - \varphi(0)\| \to 0$ as $t \to 0$. It is often important to know that for each t, M_t is a continuous operator on $\mathscr{H}$ since in applications, this says that the solutions of differential equations depend continuously on the initial data. Notice that since M_t is in general nonlinear, it is not sufficient to prove that M_t is bounded on bounded sets.

Theorem X.75 Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$ and J a nonlinear mapping on $\mathscr{H}$ satisfying $(\mathscr{H}_0^{\mathrm{L}})$. Suppose that for all k, T, solutions of (X.143) are a priori bounded, uniformly for all $\|\varphi(0)\| \leq k$, $0 < t < T$. Then each M_t is uniformly continuous on balls in $\mathscr{H}$.

Proof Let k, T be given and let $b_T(k)$ be the corresponding uniform bound. Suppose that $\|\varphi_1(0)\| \leq k$, $\|\varphi_2(0)\| \leq k$ and let $\varphi_1(t)$, $\varphi_2(t)$ be the corresponding solutions of (X.143). Then, for $t < T$,

$$\|\varphi_1(t) - \varphi_2(t)\| \leq \|\varphi_1(0) - \varphi_2(0)\| + \int_0^t \|J(\varphi_1(s)) - J(\varphi_2(s))\|\, ds$$

$$\leq \|\varphi_1(0) - \varphi_2(0)\| + C(b(k), b(k)) \int_0^t \|\varphi_1(s) - \varphi_2(s)\|\, ds$$

so,

$$\|\varphi_1(t) - \varphi_2(t)\| \leq \|\varphi_1(0) - \varphi_2(0)\| \exp(C(b(k), b(k))t) \blacksquare$$

With stronger hypothesis on J one can obtain a stronger conclusion; see Problem 80.

* * *

We now return to our motivating example, the nonlinear Klein–Gordon equation on $\mathbb{R}^3$. In that case, $B = (-\Delta + m^2)^{1/2}$ on $L^2(\mathbb{R}^3)$, $\mathscr{H} = D(B) \oplus L^2(\mathbb{R}^3)$, and

$$A = i\begin{pmatrix} 0 & I \\ -B^2 & 0 \end{pmatrix}$$

In the following, the symbol $\|\cdot\|$ will always denote the norm

$$\|\langle u, v\rangle\|^2 = \|Bu\|_2^2 + \|v\|_2^2$$

on $\mathscr{H}$ and $\|\cdot\|_p$ will denote the ordinary L^p norm on $\mathbb{R}^3$. We reformulated the Klein–Gordon equation (X.138) as

$$\begin{aligned} \varphi'(t) &= -iA\varphi(t) + J(\varphi(t)) \\ \varphi(0) &= \varphi_0 \end{aligned} \tag{X.147}$$

where $\varphi(t) = \langle u(t), v(t)\rangle$, $\varphi_0 = \langle f(x), g(x)\rangle$, $J(\varphi(t)) = \langle 0, -\lambda|u(t)|^2 u(t)\rangle$, and we showed in the proposition that A is self-adjoint on $D(B^2) \oplus D(B)$. In order to apply the abstract theory to this case we must verify that J has the right properties. No new techniques are required but just an appropriate use of Hölder's inequality, the Plancherel theorem, and a Sobolev estimate. We proceed by a series of lemmas. In all the following calculations, various universal constants will be denoted by K.

Lemma 2 Let $u \in C_0^\infty(\mathbb{R}^3)$. Then $\|u\|_6 \leq K\|Bu\|_2$.

Proof Denote $\partial u(x)/\partial x_i$ by u_{x_i}. Then by the fundamental theorem of calculus,

$$|u(x)|^4 \leq 4 \int |u_{x_i} u^3|\, dx_i$$

where the integral is taken over the line where x_j is held fixed for $j \neq i$. Thus

$$|u(x)|^6 \leq K\left(\int |u_{x_1} u^3|\, dx_1\right)^{1/2}\left(\int |u_{x_2} u^3|\, dx_2\right)^{1/2}\left(\int |u_{x_3} u^3|\, dx_3\right)^{1/2}$$

so by integrating both sides (by iterating the integrals) and using the Schwarz inequality, one obtains

$$\int_{\mathbb{R}^3}|u|^6\,dx \le K\left(\int_{\mathbb{R}^3}|u_{x_1}u^3|\,dx\right)^{1/2}\left(\int_{\mathbb{R}^3}|u_{x_2}u^3|\,dx\right)^{1/2}\left(\int_{\mathbb{R}^3}|u_{x_3}u^3|\,dx\right)^{1/2}$$
$$\le K\left(\int_{\mathbb{R}^3}|u|^6\,dx\right)^{3/4}\left(\int_{\mathbb{R}^3}|u_{x_1}|^2\,dx\right)^{1/4}$$
$$\times\left(\int_{\mathbb{R}^3}|u_{x_2}|^2\,dx\right)^{1/4}\left(\int_{\mathbb{R}^3}|u_{x_3}|^2\,dx\right)^{1/4}$$

From this one easily obtains

$$\left(\int_{\mathbb{R}^3}|u|^6\,dx\right)^{1/6} \le K(\|u_{x_1}\|_2+\|u_{x_2}\|_2+\|u_{x_3}\|_2)$$
$$= K(\|k_1\hat{u}\|_2+\|k_2\hat{u}\|_2+\|k_3\hat{u}\|_2)$$
$$\le K\|(\textstyle\sum k_i^2+m^2)^{1/2}\hat{u}\|_2$$
$$= K\|Bu\|_2 \ \blacksquare$$

Lemma 3 Suppose that $u_1, u_2, u_3 \in D(B)$. Then

$$\|u_1u_2u_3\|_2 \le K\|Bu_1\|_2\|Bu_2\|_2\|Bu_3\|_2 \tag{X.148}$$

Proof Let $u \in D(B)$. Since B is essentially self-adjoint on $C_0^\infty(\mathbb{R}^3)$, we can find a sequence of $C_0^\infty(\mathbb{R}^3)$ functions u_n so that $u_n \xrightarrow{L^2} u$ and $Bu_n \xrightarrow{L^2} Bu$, and by passing to a subsequence if necessary, we may assume u_n converges pointwise to u also. But

$$\|u_n^3-u_m^3\|_2 = \|(u_n-u_m)(u_n^2+u_nu_m+u_m^2)\|_2$$
$$\le K\|u_n-u_m\|_6\|(u_n^2+u_nu_m+u_m^2)\|_3$$
$$\le K\|u_n-u_m\|_6(\|u_n\|_6^2+\|u_n\|_6\|u_m\|_6+\|u_m\|_6^2)$$
$$\le K\|Bu_n-Bu_m\|_2(\|Bu_n\|_2^2+\|Bu_n\|_2\|Bu_m\|_2+\|Bu_m\|_2^2)$$

so $\{u_n^3\}$ is Cauchy in L^2 and since it converges pointwise to u^3 we have $u^3 \in L^2$. Taking the limit in the inequality we obtain

$$\|u\|_6^3 = \|u^3\|_2 \le K\|Bu\|_2^3$$

The statement of the lemma now follows by applying Hölder's inequality twice. ∎

Lemma 4 For all $\varphi_1, \varphi_2 \in \mathscr{H}$, J satisfies

$$\|J(\varphi_1)\| \le K\|\varphi_1\|^3$$
$$\|J(\varphi_1)-J(\varphi_2)\| \le C(\|\varphi_1\|,\|\varphi_2\|)\|\varphi_1-\varphi_2\|$$

Proof Let $\varphi_i = \langle u_i, v_i\rangle$. Then, by Lemma 3,

$$\|J(\varphi_1)\| = \|\lambda u_1^2\bar{u}_1\|_2 \le K\|Bu_1\|_2^3 \le K\|\varphi_1\|^3$$

and (by the calculation in Lemma 3)

$$\|J(\varphi_1)-J(\varphi_2)\| = \|\lambda(u_1^2\bar{u}_1-u_2^2\bar{u}_2)\|_2$$
$$\le K\|B(u_1-u_2)\|_2(\|Bu_1\|_2^2+\|Bu_1\|_2\|Bu_2\|_2+\|Bu_2\|_2^2)$$
$$\le K\|\varphi_1-\varphi_2\|(\|\varphi_1\|^2+\|\varphi_1\|\,\|\varphi_2\|+\|\varphi_2\|^2)$$

which proves the lemma. ∎

Lemma 5 Let $\varphi_1, \varphi_2 \in D(A)$, then

$$\|AJ(\varphi_1)\| \le K\|\varphi_1\|^2\|A\varphi_1\|$$
$$\|A(J(\varphi_1)-J(\varphi_2))\| \le C(\|\varphi_1\|,\|\varphi_2\|,\|A\varphi_1\|,\|A\varphi_2\|)\|A\varphi_1-A\varphi_2\|$$

Proof Let $\varphi_i = \langle u_i, v_i\rangle$ where $u_i \in D(B^2)$, $v_i \in D(B)$. We compute

$$\|Bu_{x_i}\|_2^2 = \|(\textstyle\sum k_i^2+m^2)^{1/2}k_i\hat{u}\|_2^2 \le \|(\sum k_i^2+m^2)\hat{u}\|_2^2 = \|B^2u\|_2^2$$

so, by Lemma 3,

$$\|(u^2\bar{u})_{x_i}\|_2 = \|2uu_{x_i}\bar{u}+u^2\bar{u}_{x_i}\|_2 \le K\|Bu\|_2^2\|Bu_{x_i}\|_2 \le K\|Bu\|_2^2\|B^2u\|_2$$

Thus,

$$\|AJ(\varphi_1)\|^2 = \lambda^2\|Bu_1^2\bar{u}_1\|_2^2 = \lambda^2\sum_{i=1}^3\|(u_1^2\bar{u}_1)_{x_i}\|_2^2+\lambda^2m^2\|u_1^2\bar{u}_1\|_2^2$$
$$\le K(\|Bu_1\|_2^4\|B^2u_1\|_2^2+m^2\|Bu_1\|_2^6)$$
$$\le K\|Bu_1\|_2^4\|B^2u_1\|_2^2$$
$$\le K\|\varphi_1\|^4\|A\varphi_1\|^2$$

which proves the first inequality. To prove the second, we compute by Lemma 3 and the above,

$$\tfrac{1}{4}\|(u_1^2\bar{u}_1-u_2^2\bar{u}_2)_{x_i}\|_2^2 \le \|u_1^2(\bar{u}_1-\bar{u}_2)_{x_i}\|_2^2+\|(u_1^2-u_2^2)(\bar{u}_2)_{x_i}\|_2^2$$
$$+\|2(u_1)_{x_i}(|u_1|^2-|u_2|^2)\|_2^2+\|2(u_1-u_2)_{x_i}|u_2|^2\|_2^2$$
$$\le K(\|Bu_1\|_2^4\|B^2(u_1-u_2)\|_2^2$$
$$+\|B^2u_2\|_2^2\|B(u_1+u_2)\|_2^2\|B^2(u_1-u_2)\|_2^2)$$
$$\le K(\|\varphi_1\|^4\|A(\varphi_1-\varphi_2)\|^2$$
$$+\|A\varphi_2\|^2(\|\varphi_1\|+\|\varphi_2\|)\|A(\varphi_1-\varphi_2)\|^2)$$

Therefore

$$\begin{aligned}\|A(J(\varphi_1) - J(\varphi_2))\|^2 &= \lambda^2 \|B(u_1^2\bar{u}_1 - u_2^2\bar{u}_2)\|_2^2 \\ &= \lambda^2 \sum_{i=1}^{3} \|(u_1^2\bar{u}_1 - \bar{u}_2 u_2^2)_{x_i}\|_2^2 + m^2\lambda^2\|u_1^2\bar{u}_1 - u_2^2\bar{u}_2\|_2^2 \\ &\le C(\|\varphi_1\|, \|\varphi_2\|, \|A\varphi_2\|)\|A(\varphi_1 - \varphi_2)\|^2 \\ &\quad + C(\|\varphi_1\|, \|\varphi_2\|)\|A(\varphi_1 - \varphi_2)\|^2\end{aligned}$$

which proves the lemma. We have several times used the inequality $\|Bu\|_2 \le K\|B^2u\|_2$. ∎

The last two lemmas and Theorem X.72 guarantee the local existence of a solution to (X.138). To get global existence we need:

Lemma 6 Let $u(x, t)$ be the solution of (X.138) on an interval $[0, T)$ where $u(x, 0) = f(x) \in D(B^2)$ and $u_t(x, 0) = g(x) \in D(B)$. Then

$$E(t) \equiv \frac{1}{2}\int \left\{ |Bu(x, t)|^2 + |u_t(x, t)|^2 + \frac{\lambda}{2}|u(x, t)|^4 \right\} d^3x$$

is independent of t.

Proof Let $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$. Since $\varphi(t) \in D(A)$ for each $t \in [0, T)$, we have $u(\cdot, t) \in D(B^2)$ and $u_t(x, t) \in D(B)$ for each $t \in [0, T)$. Further, since $\varphi(t)$ is strongly differentiable, u and u_t are strongly differentiable as $L^2(\mathbb{R}^3)$-valued functions and

$$\begin{aligned}\left\| B\left(\frac{u(t+h) - u(t)}{h} - u_t(t)\right) \right\|_2 &\to 0 \\ \left\| \frac{u_t(t+h) - u_t(t)}{h} - u_{tt}(t) \right\|_2 &\to 0\end{aligned} \tag{X.149}$$

as $h \to 0$. From this it follows that the first two terms in $E(t)$ are differentiable. To see that the third term is differentiable we use Lemma 2 and Hölder's inequality to conclude that

$$\begin{aligned}&\left\| u\left(\frac{u(t+h) - u(t)}{h} - u_t(t)\right) \right\|_2 \\ &\quad \le \|u\|_2^{1/2}\|Bu\|_2^{1/2} \left\| B\left(\frac{u(t+h) - u(t)}{h} - u_t(t)\right) \right\|_2\end{aligned}$$

From this and (X.149) above, it follows that $u(t, x)^2$ is strongly differentiable. Therefore

$$\int |u(t, x)|^4\, dx = (u^2(t), u^2(t))_2$$

is differentiable. Thus, $E(t)$ is differentiable and

$$\begin{aligned}E'(t) &= \frac{1}{2}(Bu_t, Bu) + \frac{1}{2}(u_{tt}, u_t) + \frac{\lambda}{2}(uu_t, u^2) \\ &\quad + \frac{1}{2}(Bu, Bu_t) + \frac{1}{2}(u_t, u_{tt}) + \frac{\lambda}{2}(u^2, uu_t) \\ &= \frac{1}{2}(u_t, B^2u + u_{tt} + \lambda|u|^2u) + \frac{1}{2}(B^2u + u_{tt} + \lambda|u|^2u, u_t) \\ &= 0\end{aligned}$$

on account of the differential equation for u. ∎

Theorem X.76a Let $\lambda > 0$, $m > 0$ and suppose

$$f \in D(-\Delta + m^2), \qquad g \in D((-\Delta + m^2)^{1/2})$$

Then there exists a unique function $u(x, t)$, $t \in \mathbb{R}$, $x \in \mathbb{R}^3$, so that $t \mapsto u(\cdot, t)$ is a twice strongly differentiable $L^2(\mathbb{R}^3)$-valued function of t, $u(\cdot, t) \in D(-\Delta + m^2)$ for all t, $u(x, 0) = f(x)$, $u_t(x, 0) = g(x)$, and

$$u_{tt} - \Delta u + m^2u = -\lambda|u|^2u \tag{X.138}$$

Moreover, for each t, the map $\langle f, g\rangle \mapsto \langle u(\cdot, t), u_t(\cdot, t)\rangle$ is continuous.

Proof Lemmas 4 and 5 show that J satisfies the hypotheses (H_0'), (H_1'), (H_0^L), and (H_1^L) of Theorem X.72. Thus, a unique local solution $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$ exists on an interval $[0, T)$. By Lemma 6, $E(t)$ is constant, so for all $t \in [0, T)$,

$$\begin{aligned}\frac{1}{2}\|\varphi(t)\|^2 &\le \frac{1}{2}\|\varphi(t)\|^2 + \frac{\lambda}{4}\int_{\mathbb{R}^3}|u(x, t)|^4\, d^3x \\ &= E(t) = E(0)\end{aligned}$$

Thus $\|\varphi(t)\|$ is bounded on $[0, T)$, so by Theorem X.74 the solution exists for all $t \ge 0$. By solving the equation with initial data $\langle f, -g\rangle$ we obtain a solution for $t \le 0$. The other statements also follow immediately from part (a) of Theorem X.73 and Theorem X.75. In verifying the hypotheses of Theorem X.75, it is necessary to note that the nonlinear term in the energy can be bounded by the square of the free energy. ∎

From a classical point of view, Theorem X.75 is not completely satisfactory. We would like to know that if we start out with initial data with a certain degree of smoothness the solution will remain that smooth. It is for this reason that one needs Theorem X.73. We will sketch the proof of the C^∞ result.

Theorem X.76b Suppose that the initial data f and g in Theorem X.76a are both in $C_0^\infty(\mathbb{R})$. Then the solution $u(x, t)$ of (X.138) is in $C^\infty(\mathbb{R}^4)$.

Proof First one proves the higher order estimates (H_n') and (H_n^{L}) for all $n > 1$. The proofs are straightforward and use exactly the same ideas that we used in proving the cases $n = 0$ and $n = 1$ in Lemmas 5 and 6. Then one verifies for each n the hypotheses on J given in part (b) of Theorem X.73. To show what is involved we will do the case $n = 2$. Suppose that $\varphi(t)$ solves (X.147), $\varphi(t) \in D(A^2)$, $\varphi'(t) \in D(A)$, and $A\varphi'(t)$ is continuous in t. We must show that $J(\varphi(t))$ is strongly differentiable. Now, $\varphi(t) = \langle u(t), u'(t)\rangle$ and by the hypotheses on φ, $u(t) \in D(B^3)$ and $u'(t) \in D(B^2)$. We can write

$$\frac{1}{h}\left(J(\varphi(t+h)) - J(\varphi(t))\right) = -\lambda\left\langle 0, \frac{|u(t+h)|^2u(t+h) - |u(t)|^2u(t)}{h}\right\rangle$$

as the sum of three terms one of which is

$$-\lambda\left\langle 0, |u(t)|^2\left(\frac{u(t+h) - u(t)}{h}\right)\right\rangle$$

and the other two are similar. By Lemma 4,

$$\left\| |u(t)|^2\left[\left(\frac{u(t+h) - u(t)}{h}\right) - u'(t)\right]\right\|_2$$

$$\leq K\|Bu(t)\|_2^2 \left\| B\left[\frac{u(t+h) - u(t)}{h} - u'(t)\right]\right\|_2$$

But, since $\varphi(t)$ is strongly differentiable, the right-hand side converges to zero. The same argument works for the other two terms so we conclude that $J(\varphi(t))$ is strongly differentiable,

$$(J(\varphi(t)))' = -\lambda\langle 0, 2u\bar{u}u' + u^2\bar{u}'\rangle$$

$(J(\varphi(t)))' \in D(A^{2-1-1}) = \mathscr{H}$ by Lemma 4 again, and $J(\varphi(t))'$ is continuous. By exactly such arguments as these one verifies the hypotheses of part (b) of Theorem X.73.

Now, since $f, g \in C_0^\infty(\mathbb{R}^3)$, $\varphi_0 = \langle f, g\rangle$ is contained in $\bigcap_{n=1}^\infty D(A^n)$. Therefore, by the Corollary to Theorem X.73, we see that $\varphi(t)$ is infinitely often strongly differentiable and for each j, the jth derivative $\varphi^{(j)}(t)$ is in $\bigcap_{n=1}^\infty D(A^n)$ for all t. All that remains is to prove that there is a function, u, C^∞ in the classical sense, so that if we view $u(\cdot, t)$ as a vector-valued function of t, then $\varphi(t) = \langle u(x, t), u_t(x, t)\rangle$. Now $u(t)$, the first component of $\varphi(t)$ is locally an element of $L^2(\mathbb{R}, L^2(\mathbb{R}^3)) = L^2(\mathbb{R}^4)$ (see Section II.4). The L^2 derivatives of u in the time direction are clearly the distributional derivatives (since $C_0^\infty \subset L^2$), and since $\partial^k u/\partial t^k \in \bigcap_{n=1}^\infty D(B^n)$ by the above argument, the distributional derivatives of u are L^2 for all orders. By Sobolev's lemma (Theorem IX.24), u is C^∞ in the classical sense. ∎

Finally, to complete our analysis of the nonlinear Klein–Gordon equation we show that the solution propagates at speed one. In particular, the solution u of the last theorem has the property that $u(\cdot, t) \in C_0^\infty(\mathbb{R}^n)$ for all t.

Theorem X.77 Let $f \in D(-\Delta + m^2)$ and $g \in D((-\Delta + m^2)^{1/2})$ and suppose that f and g are supported by a compact set $\Sigma \subset \mathbb{R}^3$ (i.e., f and g are zero a.e. outside of Σ). Then the solution of (X.138) given by Theorem X.76a has the property that $u(\cdot, t)$ is supported by

$$\mathscr{C}(\Sigma, t) = \{x \in \mathbb{R} \mid \operatorname{dist}(x; \Sigma) \leq t\}$$

Proof First we prove the statement of the theorem for the *linear* equation

$$\begin{aligned} u_{tt} - \Delta u + m^2u &= 0 \\ u(x, 0) &= f(x) \\ u_t(x, 0) &= g(x) \end{aligned} \tag{X.150}$$

Suppose first that f and g have support in S_R^0, the ball of radius R about zero. Then the solution of (X.150) is given by

$$u(t) = \cos(tB)f + B^{-1}\sin(tB)g$$

or, taking Fourier transforms,

$$\hat{u}(k, t) = \cos(t\sqrt{k^2 + m^2})\hat{f}(k) + (k^2 + m^2)^{-1/2}\sin(t\sqrt{k^2 + m^2})\hat{g}(k)$$

By the Paley–Wiener theorem (for distributions), $\hat{f}$ and $\hat{g}$ are entire analytic functions and there are constants C_i and integers N_i so that

$$|\hat{f}(k)| \leq C_1(1 + |k|^2)^{N_1}e^{|\operatorname{Im} k|R}$$
$$|\hat{g}(k)| \leq C_2(1 + |k|^2)^{N_2}e^{|\operatorname{Im} k|R}$$

Further, since the roots drop out in the power series, $\cos(t\sqrt{k^2+m^2})$ and $(k^2+m^2)^{-1/2}\sin(t\sqrt{k^2+m^2})$ are also entire and satisfy

$$|\cos(t\sqrt{k^2+m^2})| \leq C_3 e^{|\operatorname{Im} k|t}$$
$$|(k^2+m^2)^{-1/2}\sin(t\sqrt{k^2+m^2})| \leq C_4 e^{|\operatorname{Im} k|t}$$

Thus $\hat{u}(k,t)$ is entire in k and there is a constant C and an integer N so that

$$|\hat{u}(k,t)| \leq C(1+|k|^2)^N e^{|\operatorname{Im} k|(R+t)}$$

By the converse part of the Paley–Wiener theorem $u(x,t)$ therefore has support in $S^0_{R+t} = \mathscr{C}(S^0_R, t)$. From the translation invariance of the equation it follows immediately that if f and g have their support in any sphere S, then $u(x,t)$ is supported by $\mathscr{C}(S,t)$. Finally, if f and g are supported by Σ, we can, given any $\varepsilon > 0$, find a finite number of spheres $S_1, \ldots, S_M$ so that $\Sigma \subset \bigcup_{i=1}^M S_i$ and $\bigcup_{i=1}^M S_i \subset \mathscr{C}(\Sigma, \varepsilon)$. Using again the fact that the solution depends linearly on the initial data, we easily conclude that the support of $u(x,t)$ is contained in $\bigcup_{i=1}^M \mathscr{C}(S_i,t)$ which is contained in $\mathscr{C}(\Sigma, t+\varepsilon)$. Since ε was arbitrary, $u(x,t)$ is supported by $\mathscr{C}(\Sigma,t)$.

We turn now to the nonlinear problem. Suppose that in the proof of Theorem X.72, we had chosen $\tilde{X}_{T,\varepsilon,\varphi_0} = \{\varphi(\cdot) \in X_{T,\varepsilon,\varphi_0} | \operatorname{supp}\varphi(t) \subset \mathscr{C}(\Sigma,t)\}$ instead of $X_{T,\varepsilon,\varphi_0}$. Then all the estimates work as before so we need only check that

$$(S\varphi)(t) = e^{-iAt}\varphi_0 + \int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds$$

takes $\tilde{X}_{T,\varepsilon,\varphi_0}$ into itself (as far as the support property is concerned). By the result for the linear equation proven above, $e^{-iAt}\varphi_0$ has support in $\mathscr{C}(\Sigma,t)$. Further, if supp $\varphi(s) \subset \mathscr{C}(\Sigma,s)$, then

$$\begin{aligned}\operatorname{supp} J(\varphi(s)) &= \operatorname{supp}\langle 0, -\lambda|u(s)|^2u(s)\rangle \\ &\subset \operatorname{supp}\varphi(s) \subset \mathscr{C}(\Sigma,s)\end{aligned}$$

so by the linear result

$$\operatorname{supp}\{e^{-iA(t-s)}J(\varphi(s))\} \subset \mathscr{C}(\Sigma, s+(t-s)) = \mathscr{C}(\Sigma,t)$$

Thus $\int_0^t e^{-iA(t-s)}J(\varphi(s))\,ds$ is the integral of an $L^2(\mathscr{C}(\Sigma,t))$-valued function and so it too has support in $\mathscr{C}(\Sigma,t)$. Thus, S takes $\tilde{X}_{T,\varepsilon,\varphi_0}$ into itself so the unique fixed point $\varphi(t) = \langle u(x,t), u_t(x,t)\rangle$ which is our solution also has support in $\mathscr{C}(\Sigma,t)$ for each t. ∎

We conclude the section by showing that global existence does not hold in a large class of examples.

Example By applying the theorems of this section, one can easily prove local existence, uniqueness, and smoothness of solutions of the equation on $\mathbb{R}^2$:

$$\begin{aligned}u_{tt} - u_{xx} &= u^n \\ u(x,0) &= u_0(x) \\ u_t(x,0) &= v_0(x)\end{aligned} \tag{X.151}$$

where $x \in \mathbb{R}$ and $n > 1$. Further, if u_0 and v_0 are real-valued, then u is real-valued and, by the same argument as above, if u_0 and v_0 have compact support, then so will u for each t. So let u be a local solution of (X.151) where u_0 and v_0 are in $C_0^\infty(\mathbb{R})$. We will show that if u_0 and v_0 are chosen correctly, then

$$F(t) \equiv \int_{\mathbb{R}} u(x,t)^2\,dx$$

goes to infinity in finite time. Suppose that we can find an $\alpha > 0$ and initial data u_0 and v_0 so that

(A) $(F(t)^{-\alpha})'' \leq 0$ for all $t \geq 0$
(B) $(F(t)^{-\alpha})' < 0$ at $t = 0$

Then $F(t)^{-\alpha}$ will go to zero in finite time; see Figure X.8. Condition (B) is automatically satisfied by choosing u_0 and v_0 to have the same sign on $(-\infty,\infty)$ since

$$(F(0)^{-\alpha})' = -\alpha F(0)^{-1-\alpha}F'(0) = -2\alpha F(0)^{-1-\alpha}\int u_0 v_0\,dx$$

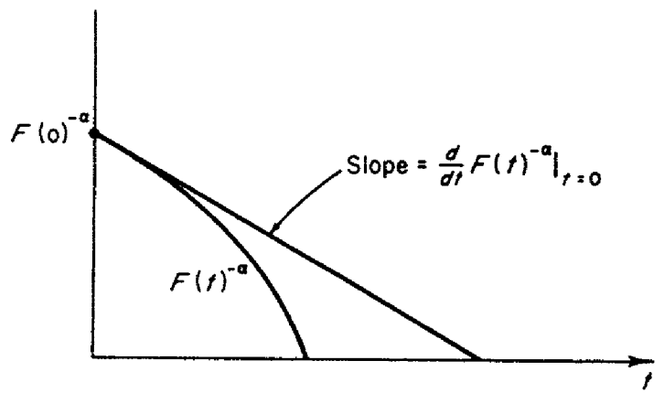


FIGURE X.8 The graph of $F(t)^{-\alpha}$.

so it remains to arrange for (A) to hold. Since $F(t) \geq 0$ this is the same as showing that $Q(t) \geq 0$ where

$$Q(t) \equiv (-\alpha)^{-1} F^{\alpha+2}(F^{-\alpha})'' = F''F - (\alpha+1)(F')^2$$

But,

$$F'(t) = 2\int uu_t\, dx$$

$$F''(t) = 2\int (uu_{tt} + u_t^2)\, dx$$

$$= 4(\alpha+1)\int u_t^2\, dx + 2\int (uu_{tt} - (2\alpha+1)u_t^2)\, dx$$

so,

$$Q(t) = 4(\alpha+1)\left\{\left(\int u^2\, dx\right)\left(\int u_t^2\, dx\right) - \left(\int uu_t\, dx\right)^2\right\}$$
$$+ 2F(t)\left\{\int uu_{tt}\, dx - \int (2\alpha+1)u_t^2\, dx\right\}$$

The first term on the right is positive by the Schwarz inequality, so we need only arrange that $H(t) \geq 0$ where

$$H(t) \equiv \int uu_{tt}\, dx - (2\alpha+1)\int u_t^2\, dx$$

$$= \int u^{n+1}\, dx + \int uu_{xx}\, dx - (2\alpha+1)\int u_t^2\, dx$$

$$= \int u^{n+1}\, dx - \int u_x^2\, dx - (2\alpha+1)\int u_t^2\, dx$$

The conserved energy for (X.151) is

$$E(t) = \frac{1}{2}\int (u_x^2 + u_t^2)\, dx - \frac{1}{n+1}\int u^{n+1}\, dx$$

That is, $E(t)$ is independent of t. Thus, if we choose α so that $2(2\alpha+1) = n+1$, we have

$$H(t) = -(n+1)E(t) + 2\alpha\int u_x^2\, dx$$

$$= -(n+1)E(0) + 2\alpha\int u_x^2\, dx \qquad \text{(X.152)}$$

Thus, if $E(0) < 0$, then H is always strictly positive since $\alpha = \frac{1}{4}(n-1) \geq 0$. Now, choosing $u_0 \geq 0$, $v_0 \geq 0$ so that (B) is satisfied, we scale u_0 by multiplying by a positive constant until $E(0) < 0$ (this will eventually happen since $n+1 > 2$). For any such initial data, $F(t)$ goes to infinity in finite time.

If we consider instead the differential equation

$$u_{tt} - u_{xx} = -u^n$$

then $H(t)$ again satisfies (X.152), but now the conserved energy is

$$E(t) = \frac{1}{2}\int (u_x^2 + u_t^2)\, dx + \frac{1}{n+1}\int u^{n+1}\, dx$$

If n is even then by choosing $u_0(x) \leq 0$, $v_0(x) \leq 0$ (thus satisfying (B)) with u_0 sufficiently large we can obtain $E(0) \leq 0$ and thus the solution blows up in finite time. If, on the other hand, n is odd, then $E(t)$ is always greater than or equal to zero so the above argument does not work. This is not surprising since the $-u^3$ case is just the one-dimensional mass zero analogue of (X.138) where we have proven global existence.

X.14 The Hilbert space approach to classical mechanics

In this final section on the existence of dynamics, we want to briefly describe the L^2 approach to classical mechanics, its comparison with quantum theory and its limitations. Throughout, we will deal with systems whose phase space is $\mathbb{R}^{6N}$ (or $\mathbb{R}^{6N}$ with some singularity sets removed) and leave the discussion of more general symplectic manifolds to the Notes.

Let us begin with the formal elements of the theory. $\mathbb{R}^{6N}$ has a distinguished coordinate system p_i, q_i $(i = 1, \ldots, 3N)$ and a point in this **phase space** moves according to the equations of motion

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}; \qquad \dot{q}_i = \frac{\partial H}{\partial p_i} \qquad \text{(X.153)}$$

where H is the energy function. In particular, a conservative Newtonian system

$$m_i \ddot{q}_i(t) = F_i(q_1, \ldots, q_{3N})$$

with

$$F_i(q) = -\frac{\partial V}{\partial q_i}$$

is of the form (X.153) if $H = \sum_{i=1}^{3N} (2m_i)^{-1} p_i^2 + V$.

(X.153) is, in general, a nonlinear ordinary differential equation in a finite-dimensional vector space. There is a standard method for rewriting such a system as a *linear* equation on an infinite-dimensional space. Namely, we transfer the action from points to functions. Let $\omega(q_0, p_0, t) = \langle q(t), p(t)\rangle$ where $\langle q(t), p(t)\rangle$ is the solution of (X.153) with initial data $q(0) = q_0$, $p(0) = p_0$. ω is a map from $\mathbb{R}^{6N+1}$ to $\mathbb{R}^{6N}$. Let

$$(U_t f)(q, p) = f(\omega(q, p; t)) \tag{X.154}$$

where f is a complex valued function on $\mathbb{R}^{6N}$. Then $U_t U_s = U_{t+s}$. We can formally compute the infinitesimal generator $i\, dU_t/dt$ by

$$\left.\frac{d(U_t f)}{dt}\right|_{t=0} = \sum_{i=1}^{3N} \frac{\partial f}{\partial q_i}\dot{q}_i + \frac{\partial f}{\partial p_i}\dot{p}_i$$
$$= \{f, H\} \tag{X.155}$$

by (X.153) where

$$\{f, g\} = \sum_{i=1}^{3N} \left(\frac{\partial f}{\partial q_i}\frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial g}{\partial q_i}\right)$$

is the Poisson bracket. Obviously,

$$\{f, g\} = -\{g, f\} \tag{X.156}$$

and an integration by parts proves that

$$\int h\{f, g\}\, dp^{3N}\, dq^{3N} = \int \{h, f\} g\, d^{3N}p\, d^{3N}q \tag{X.157}$$

if $f, g, h \in C_0^\infty(\mathbb{R}^{6N})$.

These formal preliminaries suggest the following definition:

Definition Given any locally L^1 function $H(p, q)$ on $\mathbb{R}^{6N}$, we define the **Liouville form**, a quadratic form on $L^2(\mathbb{R}^{6N}, d^{3N}p\, d^{3N}q)$, with form domain $Q(\ell) = C_0^\infty(\mathbb{R}^{6N})$ by

$$\ell(f, g) = \int \{\bar{f}, g\} H\, d^{3N}p\, d^{3N}q \tag{X.158}$$

If H is a C^1 function, we define the **Liouville operator** on $C_0^\infty(\mathbb{R}^{6N})$ by

$$Lf = \{f, H\} \tag{X.159}$$

Using (X.156) and (X.157), it is easy (Problem 78) to prove:

Proposition

(a) The Liouville form is skew-symmetric, i.e.,

$$\ell(f, g) = -\overline{\ell(g, f)} \tag{X.160}$$

(b) If H is C^1 and $f, g \in D(L)$, then

$$(f, Lg) = \ell(f, g)$$

(c) $-iL$ is a symmetric operator.

If we know *global* existence and uniqueness of solutions of the classical ordinary differential equation (X.153), we can say more:

Theorem X.78 Let H be a C^1 function. Suppose that for each q_0, p_0, there is a unique C^1 function $\omega(q_0, p_0; t)$ from $\mathbb{R}$ to $\mathbb{R}^{6N}$ obeying (X.153) with initial condition $\omega(q_0, p_0; 0) = \langle q_0, p_0\rangle$. Suppose that ω: $\mathbb{R}^{6N+1} \to \mathbb{R}^{6N}$ is a C^1 function. Then U_t is a unitary one-parameter group whose infinitesimal generator is $-i\bar{L}$. Moreover, $-iL$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{6N})$.

That U_t is unitary is known as **Liouville's theorem**.

Proof Let $D = C_0^1(\mathbb{R}^{6N})$, the C^1 functions of compact support. By an approximation of the identity argument (see the discussion in Section VIII.1), it is easy to see that $D \subset D(\bar{L})$ and that $\bar{L}f = \{f, H\}$ for any $f \in D$. Thus $\bar{L}$ is skew-symmetric on D. Now, since ω is C^1 by hypothesis, $U_t f$ is C^1 for each fixed t. Since $\omega(\cdot, \cdot; t)$ is a one-parameter group of maps of $\mathbb{R}^6$ to $\mathbb{R}^6$, $\{\langle p, q\rangle | \omega(p, q; t) \in \text{supp } f\} = \{\omega(p, q; -t) | \langle p, q\rangle \in \text{supp } f\}$ is compact if $f \in D$ as the continuous image of a compact set. Thus U_t defined as a map on D is a one-parameter group of operators from D to D. Moreover, for any f in D,

$$\left.\frac{d}{dt} U_t f\right|_{t=0} = \{f, H\} = \bar{L}f \tag{X.161}$$

To see this note that

$$t^{-1}[U_t f(q, p) - f(q, p)] - \{f, H\}(q, p)$$
$$= \frac{f(\omega(p, q; t)) - f(\omega(p, q; 0))}{t} - \sum_i \left(\frac{\partial f}{\partial q_i}\frac{\partial H}{\partial p_i} - \frac{\partial f}{\partial p_i}\frac{\partial H}{\partial q_i}\right)$$

goes to zero pointwise by the chain rule. Moreover, since f has compact support and both f and ω are uniformly Lipschitz on compact sets, we can

dominate $t^{-1}(U_t f - f)$ by an L^2 function. Thus, by the dominated convergence theorem,

$$\|t^{-1}(U(t)f - f) - \{f, H\}\|_2 \to 0$$

so we have (X.161).

It follows by the skew symmetry of L that $(d/dt)\|U_t f\|^2 = 0$ so that U_t is bounded on D and $\|U_t f\| = \|f\|$. Thus U_t extends to a unitary operator on $\mathscr{H} = L^2(\mathbb{R}^{6N})$. Since it is given by (X.154) on D and any $f \in \mathscr{H}$ can be approximated by $f_n \in D$ with $f_n \to f$ pointwise a.e., U_t is given by (X.154) on all of $\mathscr{H}$. Since $U_t f$ is continuous for $f \in C_0^1$, it is continuous on $\mathscr{H}$. Finally, by the invariance of D under U_t, (X.161), and Theorem VIII.11, $-i\bar{L}$ is essentially self-adjoint on D and $-i\bar{L}$ is the infinitesimal generator of U_t. ∎

Unfortunately, it is usually not easy to prove that the classical equations of motion have global solutions, although if V is smooth and goes to plus infinity as $|x| \to \infty$, it is clear that solution curves stay bounded so that global solutions exist. We will presently see how to prove global existence for smooth V's which do not behave too badly at infinity. However, for many V's of interest, there are singularities at finite q, and, in fact, the equations of motion break down at "collisions." The natural thing to demand in such a situation is global existence for almost all initial conditions but even this has not been done for purely Coulomb forces if $N \geq 4$. Failing this, the next thing one might try is to prove that $-iL$ is essentially self-adjoint on some suitable set, like $C_0^\infty(M)$ where M is a dense set obtained by removing singular points from $\mathbb{R}^n$. This also remains open!

It is interesting to ask why self-adjointness results are so much easier in quantum mechanics than in classical mechanics. The reasons are several; we begin with the principal one.

(1) In the usual case, where $H = p^2 + V(q)$, $-iL$ is *never* bounded from below (or above). For let

$$(\theta f)(p, q) = f(-p, q)$$

Then

$$\theta L \theta^{-1} = -L$$

which is just an expression of the fact that $\omega(-p, q; t) = \omega(p, q; -t)$ ("time reversal invariance"), or $\theta(iL)\theta^{-1} = -iL$. Thus since $-iL$ is not bounded, it cannot be semibounded. If we define C by

$$Cf = \overline{\theta f}$$

then C is a complex conjugation with $C(-iL)C^{-1} = -iL$, so $-iL$ does have self-adjoint extensions by von Neumann's theorem (Theorem X.3).

This situation should be compared with quantum mechanics where $Cf = \bar{f}$ and $CHC^{-1} = H$, but where there is no real linear θ with $\theta H \theta^{-1} = -H$ forcing H to be unbounded both above and below.

Note that in both cases: $CqC^{-1} = q$; $CpC^{-1} = -p$.

(2) There is no dependence of p and q. Thus, if V is unbounded below, so is $H(p, q)$ while the quantum-mechanical energy operator may be bounded below on account of the uncertainty principle.

(3) Only V enters in the energy operator $-\Delta + V$ while derivatives of V enter in L. Thus singularities are made worse in L, so that, e.g. in the Coulomb case, $C_0^\infty \subset D(H_{\text{quantum}})$ but $C_0^\infty \not\subset D(L)$.

We close with an elementary existence theorem for (X.153) which will imply the skew-adjointness of L in some cases; the basic idea has already been used quite often (see the Appendix to Section X.1 and Section X.13) and is a classical analogue of Nelson's commutator theorem (see Example 4 in Section X.5).

Theorem X.79 Let V be a C^2 function on $\mathbb{R}^{3N}$ with $|\text{grad } V(q)| \leq C(q^2 + 1)^{1/2}$ for a suitable constant C. Let $H(p, q) = \sum_{i=1}^{3N} a_{ij} p_i p_j + V(q)$ where a is a strictly positive definite matrix. Then for any $\langle p_0, q_0 \rangle \in \mathbb{R}^{6N}$, there is a unique C^1 function from $\mathbb{R}$ to $\mathbb{R}^{6N}$, $\omega(p_0, q_0; t)$, satisfying (X.153) with initial conditions $\langle p_0, q_0 \rangle$. Moreover, $\omega(p_0, q_0, t)$ is a C^1 map of $\mathbb{R}^{6N+1}$ to $\mathbb{R}^{6N}$.

Proof Since V is C^2, the functions on the left-hand side of (X.153) are uniformly Lipschitz and uniformly bounded on compact subsets of $\mathbb{R}^{6N}$. Thus for any A, there is a $t(A) > 0$, so that $p_0^2 + q_0^2 + 1 \leq A$ implies that we can solve (X.153) for $|t| < t(A)$; see Section V.6. Now fix $\langle p_0, q_0 \rangle$. Let $(-T_0, T_1)$ be the maximum interval on which we can solve (X.153) with initial condition $\langle p_0, q_0 \rangle$. We will show that T_1 is ∞. For suppose not. For $0 \leq t < T_1$, let

$$N(t) = p(t)^2 + q(t)^2 + 1$$

Then

$$\begin{aligned} \dot{N}(t) &= 2\dot{p}p + 2\dot{q}q \\ &\leq 2|p(t)|\,|\text{grad } V(q(t))| + 2\|a\|\,|p(t)|\,|q(t)| \\ &\leq 2(C + \|a\|)(q^2(t) + 1)^{1/2}|p(t)| \\ &\leq (C + \|a\|)N(t) \end{aligned}$$

Thus $N(t) \leq N(0) \exp[(C + \|a\|)t]$ for all $t > 0$. Let t_0 be the $t(A)$ for $A = N(0) \exp[(C + \|a\|)T_1]$. Choose $t \in (T_1 - t_0, T_1)$. Then we can solve (X.153) with initial condition $\langle p(t), q(t) \rangle$. By piecing this solution onto the supposed maximal solution, we obtain a solution in $(-T_0, t + t_0)$ contradicting maximality. Thus $T_1 = \infty$ and similarly $T_0 = \infty$.

By the method of Section X.13, ω is C^1 in the region obtained by one application of the contraction mapping principle. By the above argument, any t can be reached by finitely many applications of the contraction mapping principle (with successively larger starting times). ∎

Corollary Under the hypotheses of Theorem X.79, the Liouville operator L is essentially skew adjoint on $C_0^\infty(\mathbb{R}^6)$, i.e. $L^{**} = -L^*$.

NOTES

Section X.1 The main theorem of this section (Theorem X.2) was proven by J. von Neumann in "Allgemeine Eigenwerttheorie Hermitescher Funktionaloperatoren," *Math. Ann.* **102** (1929–1930) 49–131. The proof that we give is due to N. Dunford and J. Schwartz, *Linear Operators*, Vol. II, Wiley (Interscience), New York, 1963, who remark that their proof has many elements in common with the approach in J. Calkin, "Abstract symmetric boundary conditions," *Trans. Amer. Math. Soc.* **45** (1939) 369–442. The original approach of von Neumann makes extensive use of the *Cayley transform* of a symmetric operator A; this is formally defined by $V = (A - i)(A + i)^{-1}$. Some aspects of the proof become more transparent in the Cayley transform language, but the connection with boundary value problems is then not so clear. The main elements of the Cayley transform proof are: (i) V is defined as a map from $\overline{\text{Ran}(A + i)}$ to $\overline{\text{Ran}(A - i)}$ and can be shown to be a partial isometry, (ii) the deficiency indices of A are precisely the codimensions of the initial and final subspaces for V, (iii) closed symmetric extensions of A are in a one-to-one correspondence with extensions of V which are partial isometries. The self-adjoint extensions are in a one-one correspondence with unitary extensions of V. Unitary extensions of V are clearly characterized by an arbitrary unitary map from $D(V)^\perp$ to $\text{Ran}(V)^\perp$. One thereby obtains the fact that self-adjoint extensions of A exist only if $D(V) = \overline{\text{Ran}(A + i)}$ and $\text{Ran}(V) = \overline{\text{Ran}(A - i)}$ have equal codimension n, and the fact that the extensions are naturally parametrized by unitary maps from one n-dimensional space to another. For additional discussion of the extension theory from this Cayley transform point of view, see N. Akhiezer and I. Glazman, *Theory of Linear Operators in Hilbert Space*, Vol. II, Ungar, New York, 1963. There is further discussion of the "physical importance" of self-adjointness in A. S. Wightman, "Introduction to some aspects of the relativistic dynamics of quantized fields," *High Energy Electromagnetic Interactions and Field Theory* (M. Levy, ed.), Gordon and Breach, New York, 1967. For references for the moment problem, see the notes to Section X.6.

There is an alternative proof of Theorem X.3 which is essentially due to A. Galindo, "On the existence of J-self-adjoint extensions of J-symmetric operators with adjoint," *Comm. Pure Appl. Math.* **15** (1962), 423–425. We will sketch the proof which avoids the theory of self-adjoint

extensions (at the cost of using Zorn's lemma). Let A satisfy the hypotheses of Theorem X.3. Then, by Zorn's lemma, A has an extension B which satisfies the following three properties:

(i) $CB = BC$
(ii) $B \subset B^*$
(iii) B is maximal with respect to conditions (i) and (ii).

Suppose that $B \neq B^*$. Then we can find a nonzero $\langle \varphi, \psi \rangle \in \mathscr{H} \oplus \mathscr{H}$, so that

(iv) $\langle \varphi, \psi \rangle \in \Gamma(B^*) \cap \Gamma(B)^\perp$

Since $C \oplus C$ leaves both $\Gamma(B)$ and $\Gamma(B^*)$ invariant (by (i)), $\langle (I + C)\varphi, (I + C)\psi \rangle$ and $\langle i(I - C)\varphi, i(I - C)\psi \rangle$ are both in $\Gamma(B^*) \cap \Gamma(B)^\perp$ and at least one of them is nonzero. We can thus suppose that

(v) $\langle C\varphi, C\psi \rangle = \langle \varphi, \psi \rangle$

Let $\tilde{\Gamma} = \Gamma(B) \oplus \{\alpha \langle \varphi, \psi \rangle \mid \alpha \in \mathbb{C}\}$. Since $\tilde{\Gamma} \subset \Gamma(B^*)$, $\tilde{\Gamma}$ is the graph of an operator $\tilde{B}$. Because $C \oplus C$ leaves $\tilde{\Gamma}$ pointwise invariant, $\tilde{B}$ obeys (i). Moreover, since $\langle \varphi, \psi \rangle \in \Gamma(B)^\perp$, we have that for any $\eta \in D(B)$

$$(\varphi + \eta, \tilde{B}(\varphi + \eta)) = (\varphi, \psi) + (\eta, B\eta)$$

By (v), (φ, ψ) is real and, by (ii), $(\eta, B\eta)$ is real so $\tilde{B}$ is symmetric. Since this contradicts (iii), we conclude that $B = B^*$ and A has self-adjoint extensions.

Incidentally, the above proof shows that under the hypotheses of Theorem X.3, A has self-adjoint extensions commuting with C, a fact which also follows from a detailed analysis of the extensions of A. The existence of such extensions is important because it implies that *on a real Hilbert space every symmetric operator has self-adjoint extensions*. For $\mathscr{H} = \mathscr{H}_{\mathbb{R}} \oplus \mathscr{H}_{\mathbb{R}}$ can be viewed as a complex Hilbert space with $i\langle \varphi, \psi \rangle = \langle -\psi, \varphi \rangle$. Letting $C\langle \varphi, \psi \rangle = \langle \varphi, -\psi \rangle$, we see that every complex linear operator on $\mathscr{H}$ commuting with C is of the form $A \oplus A$ where $A: \mathscr{H}_{\mathbb{R}} \to \mathscr{H}_{\mathbb{R}}$. This fact, together with the strong form of Theorem X.3 yields the claimed fact about symmetric operators on real Hilbert spaces. For a further discussion, see Problem 81.

The discussion in the Appendix follows the general outline of unpublished lectures of E. Nelson. Further discussion of the self-adjointness of ordinary differential operators may be found in E. Coddington and N. Levinson, *Theory of Ordinary Differential Equations*, McGraw-Hill, New York, 1955 and in Chapter XIII of the book of Dunford and Schwartz mentioned above.

Extensive historical notes on the development of this self-adjointness theory may be found in Volume II of Dunford and Schwartz; we limit ourselves to mentioning that the limit point-limit circle theory (Theorems X.6 and X.7) is due to H. Weyl who introduced many of the ideas critical to the theory of extensions of unbounded operators many years before the development of the general theory of von Neumann. See H. Weyl, "Über gewöhnliche lineare Differentialgleichungen mit singulären Stellen und ihre Eigenfunktionen," *Nachr. Akad. Wiss. Göttingen Math.-Phys. Kl. II* (1909), 37–63, and (1910), 442–467; "Über gewöhnliche Differentialgleichungen mit Singularitäten und die zugehörigen Entwicklungen willkürlicher Funktionen," *Math. Ann.* **68** (1910), 220–269. These papers can also be found in *Gesammelte Abhandlungen*, Vol. I, Springer-Verlag, Berlin, 1968.

The limit point–limit circle terminology arose from the idea of considering the self-adjointness problem for $-d^2/dx^2 + V(x)$ on (a, ∞) as a limit of problems on the interval (a, b) as $b \to \infty$. Let φ and ψ be the solutions of $-\varphi''(x) + V(x)\varphi(x) = i\varphi(x)$ on (a, ∞)

obeying $\varphi(a) = \psi'(a) = 0$, $-\varphi'(a) = \psi(a) = 1$. For fixed b, the set of $z \in \mathbb{C}$ for which $\eta = \varphi + z\psi$ obeys $(\cos\alpha)\eta(b) + (\sin\alpha)\eta'(b) = 0$ for some $\alpha \in [0, 2\pi)$ form a circle C_b. As $b \to \infty$, this circle either converges to a limiting circle or shrinks to a limiting point. In the former case, both solutions of $-\varphi''(x) + V(x)\varphi(x) = i\varphi(x)$ are L^2 near ∞; in the latter case, only one. This approach is further discussed in Coddington and Levinson.

Theorem X.8 appeared in N. Levinson, "Criteria for the limit-point case for second order linear differential operators," *Časopsis Pěst. Math. Fys.* **74** (1949) 17–20. We note that Theorem X.7 has an analogue for more general intervals than $[0, \infty)$; namely, if $V(x)$ is continuous on (a, b) with $-\infty \le a < b \le \infty$, then $-d^2/dx^2 + V(x)$ is in the limit point case at both a and b if and only if $-d^2/dx^2 + V(x)$ is essentially self-adjoint on $C_0^\infty(a, b)$. In particular, one can use Theorem X.8 to provide another proof of Problem 24 in the one-dimensional case. Theorem X.9 is due to A. Wintner in "On the Normalization of Characteristic Differentials in Continuous Spectra," *Phys. Rev.* **72** (1947) 516–517, and "The Schwartzian derivative and the approximation method of Brillouin," *Quart. Appl. Math.* **16** (1958), 82–86. A proof of Wintner's criterion and a variety of alternative criteria can be found in Dunford and Schwartz, Vol. II. The limit point case of Theorem X.10 is due to K. Friedrichs, "Über die ausgezeichnete Randbedingung in der Spektraltheorie der halbbeschränkten gewöhnlichen Differentialoperatoren zweiter ordnung," *Math. Ann.* **112** (1935/36), 1–23, and the limit circle part is due to D. Sears, "On the solutions of a linear second order differential equation which are of integrable square," *J. London Math. Soc.* **24** (1949), 207–215. Our proof is related to a general method of H. Kurss, "A limit-point criterion for non-oscillatory Sturm–Liouville differential operators," *Proc. Amer. Math. Soc.* **18** (1967), 445–449 (see Problem 8).

The first examples of potentials which are classically incomplete but quantum-mechanically complete were given in the 1949 Sears paper quoted above. The examples which we use are taken from J. Rauch and M. Reed, "Two examples illustrating the differences between classical and quantum mechanics," *Comm. Math. Phys.* **29** (1973), 105–111, and are based on suggestions of E. Nelson. H. Kalf has kindly sent to the authors his detailed analysis of Sears' example. Let V_{ab} be the potential on $(0, \infty)$ given by

$$V_{ab}(x) = \frac{2}{x^2} - 9x^4(a - 2b\cos(2x^3))$$

where a and b are in $(0, \infty)$. Then $-\varphi'' + V_{ab}\varphi = 0$ is the Mathieu equation whose general solution is

$$\frac{1}{x}\left(c_1 e^{\mu x^3}\varphi_{ab}(x^3) + c_2 e^{-\mu x^3}\varphi_{ab}(-x^3)\right)$$

where the exponent μ depends on a and b and $\varphi_{ab}(x)$ is a C^∞ function of period π unless $\langle a, b\rangle$ corresponds to a point on one of the curves in Figure X.9. The exponent μ is purely imaginary for $\langle a, b\rangle$ in the white regions of the figure and real for $\langle a, b\rangle$ in the shaded regions. V_{ab} is clearly both quantum-mechanically and classically complete at zero. At infinity, V_{ab} is quantum-mechanically complete if $\langle a, b\rangle$ falls in the shaded region since in that case μ is real so one solution is not in L^2 near infinity. However, if $\langle a, b\rangle$ is in the white region, then both solutions are in L^2 near infinity so V_{ab} is quantum-mechanically incomplete. Classically, if $2b < a$, then $V_{ab}(x) \le -dx^4$ near infinity so a classical particle can escape to infinity in finite time, that is, V_{ab} is classically incomplete. On the other hand, if $2b > a$, then the peaks in the potential grow higher and higher so V is classically complete. For information about Mathieu functions, consult N. McLachlan, *Theory and Applications of Mathieu functions*, Oxford Univ. Press, London and New York, 1947, pp. 40, 98, or

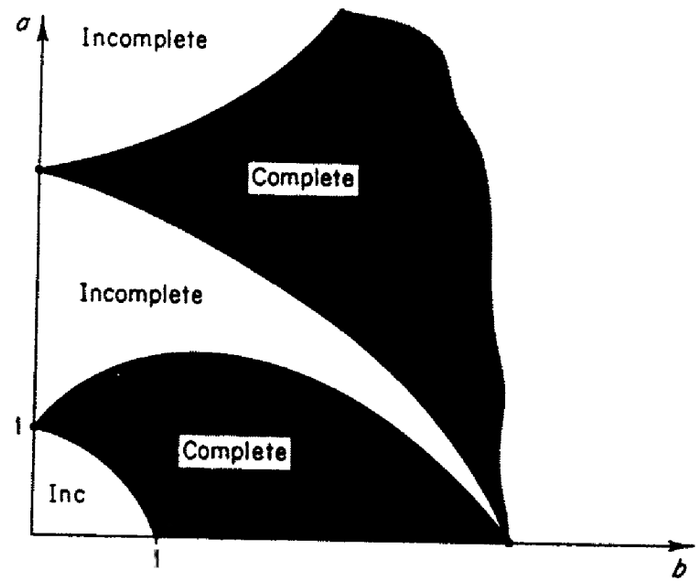


FIGURE X.9 Quantum-mechanical completeness for V_{ab}.

J. Meixner and F. Schäfke, *Mathieusche Funktionen und Sphäroidfunktionen*, Springer-Verlag, Berlin, 1954, p. 132.

Many of the criteria of essential self-adjointness of ordinary differential operators which can be derived from the Weyl theory can be generalized to partial differential operators. There is an analogue of Proposition 2 which plays an important role in these generalizations; this analogue is a theorem of E. Weinholtz, "Bemerkungen über elliptische Differentialoperatoren," *Arch. der Math.* **10** (1959), 126–133, and N. Nilsson, "Essential self-adjointness and the spectral resolution of Hamiltonian operators," *Kungl. Fys. Sällsk. i Lund Förh* **29**, (1959). These techniques played a role in various multidimensional extensions of Theorem X.8 (see the Notes to Section X.5).

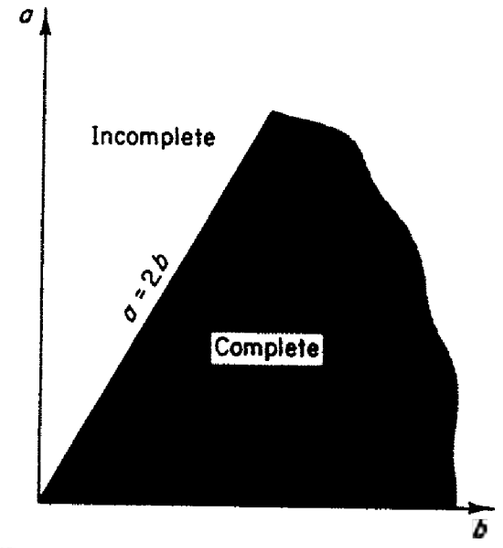


FIGURE X.10 Classical completeness for V_{ab}.

In many cases, the results obtainable by using the Weyl limit point–limit circle methods can be obtained more easily and in more generality by using the techniques of Sections X.4 and X.5.

The examples we discussed, where the classical and quantum mechanical conditions for completeness agree, required global conditions, i.e. conditions everywhere. But one would expect that a particle could be quantum mechanically trapped by a set of wide enough barriers, independent of what happens in between. A typical example in the one-dimensional case is the following theorem of R. S. Ismagilov, "Conditions for self-adjointness of differential operators of higher order," *Soviet Math.* **3** (1962), 279–283.

Theorem Let $V(x)$ be a continuous function $[0, \infty)$ and suppose there is a sequence of intervals (a_n, b_n), $b_n < a_{n+1}$, so that

(a) $V(x) \geq -(b_n - a_n)^{-2}$ for $x \in (a_n, b_n)$
(b) $\sum_n (b_n - a_n)^2 = \infty$

Then $-(d^2/dx^2) + V(x)$ is in the limit point case at infinity independent of the behavior of V outside of the intervals (a_n, b_n).

Notice that conditions (a) and (b) imply that the classical travel time across the union of the intervals (a_n, b_n) is infinite.

The first results of this general type requiring bounds only on intervals are due to P. Hartman, "The number of L^2-solutions of $x'' + q(t)x = 0$," *Amer. J. Math.* **43** (1951), 635–645. Other one-dimensional results can be found in M. S. P. Eastham, "On a limit-point method of Hartman," *Bull. London Math. Soc.* **4** (1972), 340–344, and N. P. Kupeov, "Conditions for non-self adjointness of a second order linear differential operator," *Soviet Math.* **2** (1961), 710–713. Theorems of this type applicable to noncentral potentials in many dimensions can be found in M. S. P. Eastham, W. D. Evans, and J. B. McLeod, "The Essential Self-Adjointness of Schrödinger-Type Operators," *Arch. Rational Mech. Anal.*, to appear. These authors also present examples of conditions in V in a tube $\Omega \times [0, \infty) \subset \mathbb{R}^n$ (Ω bounded and open in $\mathbb{R}^{n-1}$) so that if V obeys these conditions, then $-\Delta + V$ is not essentially self-adjoint on C_0^∞ independent of the behavior of V outside the tube. Intuitively in this case, the particle travels to infinity in the tube in finite time.

For a discussion of the Laplace–Beltrami operator used in Example 6, consult C. Müller, "Spherical Harmonics," Springer-Verlag *Lecture Notes in Mathematics* **17** (1966). In two dimensions, $B = d^2/d\theta^2$, $k_\ell = -\ell^2$, and there are two eigenfunctions corresponding to each $\ell > 0$, namely $e^{\pm i\ell\theta}$ and just the constant function corresponding to $\ell = 0$. The self-adjointness statement follows from the fact that $\{e^{i\ell\theta}\}_{\ell=-\infty}^{\infty}$ form a basis for $L^2(0, 2\pi)$. In three dimensions,

$$(Bg)(\theta, \phi) = (\sin\theta)^{-1}\left[\frac{\partial}{\partial\theta}(\sin\theta)\frac{\partial g}{\partial\theta} + \frac{\partial}{\partial\phi}(\sin\theta)^{-1}\frac{\partial g}{\partial\phi}\right]$$

where θ and ϕ are the usual angular variables in spherical coordinates. In this case $k_\ell = -\ell(\ell+1)$ and the corresponding eigenspace has dimension $2\ell + 1$. In s dimensions, $k_\ell = -\ell(\ell + s - 2)$. There is a close connection between B and the representation theory of the group $SO(s)$. In particular, there is a connection between the completeness of the eigenfunctions of B and the Peter–Weyl theorem (see Chapter XIV).

Section X.2 Theorem X.12 is due to F. Rellich: "Störungstheorie der Spektralzerlegung, II," *Math. Ann.* **116** (1939) 555–570. A wide variety of applications and extensions of the Kato–Rellich theorem can be found in the book, T. Kato, *Perturbation Theory for Linear Operators*, Springer, New York, 1966. In particular, Theorem X.13 and the special case of Theorem X.14 where (X.21a) is replaced with the stronger condition (X.21b) (equivalently (X.21c)) appear in Kato's book. Theorem X.14 is due to R. Wüst, "Generalizations of Rellich's theorem on perturbations of (essentially) self-adjoint operators," *Math. Z.* **119** (1971) 276–280; for additional discussion, see R. Wüst, "Holomorphic operator families and stability of self-adjointness," *Math. Z.* **125** (1972), 349–358.

Kato's application of Rellich's theorem to atomic Hamiltonians appeared in T. Kato, "Fundamental properties of Hamiltonian operators of Schrödinger type," *Trans. Amer. Math. Soc.* **70** (1951), 195–211. This paper was a turning point in mathematical physics for two reasons. Firstly, the proof of self-adjointness was a necessary preliminary to the problems of spectral analysis and scattering theory for these operators, problems which have occupied mathematical physicists ever since. Secondly, the paper focused attention on specific systems rather than foundational questions.

The KLMN theorem in various forms is due to T. Kato, "Quadratic forms in Hilbert space and asymptotic perturbation series," Technical report No. 7, Univ. of Calif. (1955); J. Lions, *Équations Differentielles Operationelles et Problèmes aux Limites*, Springer-Verlag, Berlin, 1961, Chapter II, Section 1; and P. Lax and A. Milgram, "Parabolic equations," in *Contributions to the theory of partial differential equations*, *Ann. Math. Study* **33**, Princeton, New Jersey, 1954. The interpretation of the theorem in terms of scales of spaces was first emphasized by E. Nelson, "Interaction of nonrelativistic particles with a quantized scalar field," *J. Math. Phys.* **5** (1964) 1190–1197.

Written in terms of operator inequalities, Theorem X.18 is slightly weaker than the statement "If $0 \leq A^2 \leq B^2$, then $0 \leq A \leq B$" which is known as the monotonicity of the square root. This is a special case of the following theorem of K. Löwner, "Über monotone Matrixfunktionen," *Math. Z.* **38** (1934), 177–216:

Theorem A necessary and sufficient condition for a continuous real-valued function f on $(0, \infty)$ to have the property that $f(A) \leq f(B)$ for all pairs of self-adjoint operators, A, B with $0 < A \leq B$ is that f be the restriction to $(0, \infty)$ of a function f analytic in $\mathbb{C}\backslash(-\infty, 0]$ with the property $(\operatorname{Im} f) \geq 0$ for all z with $\operatorname{Im} z > 0$.

The "physical" argument behind the expectation that quantum mechanics can be developed for potentials with $r^{-\alpha}$ singularities $0 < \alpha < 2$ is based on the following heuristics: First, the basic property required for a nonpathological physics is the semiboundedness of $H_0 + V$; secondly, if a wave function is concentrated in a region of size Δr about a negative $r^{-\alpha}$ singularity, then by the uncertainty principle, the expectation value of H_0 is on the order of $(\text{const})(\Delta p)^2 \approx (\text{const})(\Delta r)^{-2}$ while the expectation value of V is on the order of $(\text{const})(\Delta r)^{-\alpha}$. Since $cx^{-2} - dx^{-\alpha}$ ($c, d > 0$) is semibounded only if $0 < \alpha \leq 2$, we expect reasonable physics to break down at $\alpha = 2$.

The inequality that we have dubbed the uncertainty principal lemma is classical; see for example H. Kalf and J. Walter, "Strongly singular potentials and essential self-adjointness of singular elliptic operators in $C_0^\infty(\mathbb{R}^n\backslash\{0\})$," *J. Functional Analysis* **10** (1972), 114–130, where historical remarks are given. That $r^{-2} < -c\Delta$ for some constant is a special case of a theorem of the same type as Theorem X.21: If $s > 3$ and $V \in L^{s/2}_w$, then V is Δ-form bounded with bound less than or equal to $c\|V\|_{s/2,w}$.

The development of much of the operator theory needed for the quantum mechanics of Hamiltonians with Rollnik potentials and in particular the proof of Theorem X.19 may be found in B. Simon, *Quantum Mechanics for Hamiltonians Defined as Quadratic Forms*, Princeton Univ. Press, Princeton, New Jersey, 1971. The reader can also find there a summary of the discovery and rediscovery of the Rollnik condition by various authors.

The extension of Kato's theorem to n dimensions has been discussed by a variety of authors. Theorem X.20 appeared in F. Brownell, "A note on Kato's uniqueness criterion for Schrödinger operator selfadjoint extensions," *Pacific J. Math.* **9** (1959), 953–973; our proof of it is borrowed from an appendix of E. Nelson, "Feynman integrals and the Schrödinger equation," *J. Math. Phys.* **5** (1964) 332–343. A closely related discussion of n-dimensional potentials already appeared in F. Stummel, "Singuläre elliptische Differentialoperatoren in Hilbertschenräumen," *Math. Ann.* **132** (1956) 150–176. Stummel's results were not stated in terms of L^p spaces but in terms of conditions of the form:

$$\int_{|x-y|\leq 1} |x-y|^{-s+4-\alpha} |V(y)|^2 \, dy \leq C \qquad \text{for all } x$$

for some $\alpha > 0$. In much of the literature on Schrödinger operators, these "Stummel conditions" and the related "Stummel spaces" Q_α are used.

A direct proof of the extension of Theorem X.20 to the boundary case $p = s/2$ ($s \geq 5$) was given in W. Faris, "The product formula for semi-groups defined by Friedrichs extensions," *Pacific J. Math.* **22** (1967) 47–70. His proof uses the Sobolev embedding theorem which is in turn based on the classical Sobolev inequality discussed in Section IX.4. Strichartz' theorem in a slightly different form appears in R. Strichartz, "Multipliers on Fractional Sobolev spaces," *J. Math. Mech.* **16** (1967), 1031–1060. The applicability of this theorem to Schrödinger operators is an unpublished remark of Nelson.

That r^{-2} is a Δ-bounded perturbation on $\mathbb{R}^s$ if $s \geq 5$ follows from an explicit operator estimate of classical form: if $u \in C_0^\infty(\mathbb{R}^s \backslash \{0\})$ and if $a \geq -\frac{1}{2}s(s-4)$, then

$$\int |\Delta u|^2 \, d^s x \geq -a \int \frac{|\nabla u|^2}{|x|^2} \, d^s x + \frac{(s-4)^2}{16} (s^2 + 4a) \int \frac{|u|^2}{|x|^4} \, d^s x$$

This inequality of Rellich's is proven in F. Rellich, *Perturbation theory of eigenvalue problems*, Gordon and Breach, New York, 1969; see also the paper of Schmincke quoted below.

Konrady's trick and its application to the field theory generalization of the anharmonic oscillator appear in J. Konrady, "Almost positive perturbations of positive self-adjoint operators," *Comm. Math. Phys.* **22** (1971), 295–299. At about the same time, the same method was independently discovered in U.-W. Schmincke, "Essential self-adjointness of a Schrödinger operator with strongly singular potential," *Math. Z.* **124** (1972), 47–50.

Section X.3 In his original paper on self-adjoint extensions (see the Notes to Section X.1), von Neumann proved that a semibounded operator has semibounded extensions whose lower bound is arbitrarily close to the bound of the original operator. He conjectured that extensions exist with the same lower bound. This fact, i.e. Theorem X.23, was proven by K. Friedrichs in "Spektraltheorie halbbeschränkter Operatoren," *Math. Ann.* **109** (1934), 465–487, and by M. Stone in *Linear Transformations in Hilbert Spaces and their Applications in Analysis*, Amer. Math. Soc. Colloquium Publication **15**, Providence, Rhode Island, 1932. For further discussion of when the Friedrichs extension is the unique extension with the same lower bound (Example 1), see E. T. Poulsen, "The minimax principle and uniqueness of the Friedrichs extension," *Proc. Amer. Math. Soc.* **21** (1969), 508–509. Theorem X.24 and the proposition preceding it are due to M. Krein, "The theory of self-adjoint extensions of semibounded Hermitean operators and its applications, I," *Mat. Sb.* **20** (1947), 431–495, and is further discussed in B. Simon, "The theory of semi-analytic vectors: a new proof of a theorem of Masson and McClary," *Indiana Univ. Math. J.* **20** (1971), 145–151.

Theorem X.25 was first proven in J. von Neumann, "Uber adjungierte Funktionaloperatoren," *Ann. Math.* **33** (1932), 249–310.

Section X.4 Kato's inequality is due to T. Kato, "Schrödinger Operators with Singular Potentials," *Israel J. Math.* **13** (1973), 135–148. Theorem X.28 and X.29 also appear there. Kato was motivated in part by B. Simon, "Essential self-adjointness of Schrödinger operators with positive potentials," *Math. Ann.* **201** (1973), 211–220. Simon had proven Theorem X.28 under the stronger hypothesis $V \geq 0$, $V \in L^2(\mathbb{R}^n, \exp(-ax^2)\, d^n x)$ for some a. Previous to Simon's work, it was a folk belief that V had to be in a local Stummel space (essentially that V be in L^p_{loc} for some $p > n/2$ if $n \geq 4$) if $-\Delta + V$ was to be essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

Weaker versions of Theorem X.28 are quite old. In particular, that $-\Delta + V$ is essentially self-adjoint if $V \geq 0$ and $V \in C_0^\infty(\mathbb{R}^n)$ is a result of T. Carleman, "Sur la théorie mathématique de l'équation de Schrödinger," *Ark. Mat., Ast., Fys.* **24B**, No. 11 (1934). His result was independently rediscovered by A. Jaffe, "A $\lambda\varphi^4$ Cutoff Field Theory," Princeton Univ. thesis, Princeton, New Jersey, 1965. The extension to some classes of singular positive V was first accomplished by F. Stummel (see the Notes to Section X.2). Perhaps the strongest version of the result preceding Kato's paper appeared in H. Stetkaer-Hansen, "A generalization of a theorem of Wienholtz concerning essential self-adjointness of singular elliptic operators," *Math. Scand.* **19** (1966), 108–112 and J. Walter, "Note on a paper by Stetkaer-Hansen concerning essential self-adjointness of Schrödinger operators," *Math. Scand.* **25** (1969), 94–96, who proved a stronger result if $n \leq 3$ and a weaker theorem if $n \geq 4$.

Theorem X.30 appears in B. Simon, "Essential Self-Adjointness of Schrödinger-Operators with Singular Potentials: A Generalized Kalf-Walter-Schmincke Theorem," *Arch. Rational Mech. Anal.* **52** (1973), 44–48. A partially alternative proof can be found in H. Kalf and J. Walter, "Note on a paper of Simon on the essential self-adjointness of Schrödinger operators with singular potentials," *Arch. Rational Mech. Anal.* **52** (1973), 258–260. Simon's result generalizes results of H. Kalf and J. Walter, "Strongly singular potentials and essential self-adjointness of singular elliptic operators on $C_0^\infty(\mathbb{R}^n \backslash \{0\})$," *J. Functional Analysis* **10** (1972), 114–130, and of U.-W. Schmincke, "Essential self-adjointness of a Schrödinger operator with strongly singular potential," *Math. Z.* **124** (1972), 47–50. The earliest results of the genre are due to K. Jörgens, "Wesentliche Selbstadjungiertheit singulärer elliptischer Differentialoperatoren zweiter Ordnung in $C_0^\infty(G)$," *Math. Scand.* **15** (1964), 5–17.

Theorem X.31 is due to W. Faris, "Essential self-adjointness of operators in ordered Hilbert space," *Comm. Math. Phys.* **30** (1973), 23–34. A slightly weaker theorem was proven earlier by E. B. Davies, "Properties of the Green's functions of some Schrödinger operators," *J. London Math. Soc.* 7 (2) (1973), 473–491.

The first comprehensive treatment of Schrödinger operators with magnetic fields appears in T. Ikebe and T. Kato, "Uniqueness of the self-adjoint extension of singular elliptic differential operators," *Arch. Rational Mech. Anal.* **9** (1962), 77–92. They proved a theorem like Theorem X.34 but with stronger conditions on V. Theorem X.34 is from Kato's *Israel Journal* article. Kato proved Theorem X.33 under the weaker condition that $u \in L^1_{\text{loc}}$. We have simplified the proof by noting that $u \in L^2_{\text{loc}}$ is sufficient in applications. This remark is critical for the proof of Theorem X.35 which can be found in B. Simon, "Schrödinger operators with singular magnetic vector potentials," *Math. Z.* **131** (1973), 361–370. Simon's paper is based on a strengthened version of the technical lemma for Theorem X.33. Results similar to Theorem X.35 may be found in M. Schechter, *Spectra of Partial Differential Operators*, North-Holland, Amsterdam, 1971. Previous to Simon's paper, the use of Coulomb gauge was advocated by K. Jörgens, "Uber das wesentliche Spektrum elliptischer Differentialoperatoren vom Schrödinger-Typ," Tech. report, Univ. Heidelberg, 1965, and "Zur Spektraltheorie der Schrödingeroperatoren," *Math. Z.* **96** (1967), 355–372.

Theorem X.32 is due to T. Kato, "A second look at the essential self-adjointness of the Schrödinger operators," to appear.

Earlier results describing the domain of the Friedrichs extension can be found in K. Friedrichs, "Spektraltheorie halbbeschränkter Operatoren und Anwendung auf die Spektralzerlegung von Differentialoperatoren, II," **109** (1933/34), 685–713 (corrections in *Math. Ann.* **110** (1934/35), 777–779), and "Uber die ausgezeichnete Randbedingung in der Spektraltheorie der halbbeschränkter gewöhnlichen Differentialoperatoren zweiter Ordnung," *Math. Ann.* **112** (1935/36), 1–23; H. Freudenthal, "Über die Friedrichysche Fortsetzung halbbeschränkter Hermitescher Operatoren," *Nederl. Akad. Wetensch. Proc. Ser.* **39** (1936), 832–833; F. Rellich, "Halbbeschränkte gewöhnliche Differentialoperatoren zweiter Ordnung," *Math. Ann.* **122** (1950/51), 343–368; H. Kalf, "On the characterization of the Friedrichs extension of ordinary or elliptic differential operators with a strongly singular potential," *J. Functional Analysis* **10** (1972), 230–250.

Section X.5 Nelson's commutator theorem appeared in E. Nelson, "Time-ordered operator products of sharp-time quadratic forms," *J. Functional Analysis* **11** (1972), 211–219. Earlier a similar theorem appeared in J. Glimm and A. Jaffe, "The $\lambda(\varphi^4)_2$ quantum field theory without cutoffs, IV: Perturbation of the Hamiltonian," *J. Math. Phys.* **13** (1972), 1568–1584. The Glimm–Jaffe theorem was weaker in that bounds on both the commutator and double commutator were needed. Both Nelson and Glimm–Jaffe intended the theorem for application to the self-adjointness of smeared quantum field operators by the scheme used in Example 3. Nelson's paper also contained Lemmas 1 and 2.

Both the Nelson paper and the Glimm–Jaffe paper have somewhat more complicated proofs than the one we use and both use the not-quite-standard techniques of mollifiers and graph limits respectively. The simple proof that we use, based on the fundamental criterion, was noted by W. Faris and R. Lavine, "Commutators and self-adjointness of Hamiltonian operators," *Comm. Math. Phys.* **35** (1974), 39–48. They also give a proof based on the intuition of Example 4 and applied the theory to Schrödinger operators (Theorem X.38 and its corollaries) and to Dirac operators.

An alternative proof and a slightly more general result appear in O. McBryan, "Local generators for the Lorentz group in the $P(\varphi)_2$ model," *Nuovo Cimento* **18A** (1973), 654–662.

In Stummel's 1956 paper (see the Notes to Section X.2), the Hamiltonian of the hydrogen atom in an asymptotically constant electric field is proven essentially self-adjoint. More general atoms in constant fields were first treated in the Ikebe–Kato paper (see the Notes to Section X.4). Earlier, operators of the form $-\Delta + V$ with V *continuous* and $V(x) \geq -cx^2 - d$ were proven essentially self-adjoint on C_0^∞ by N. Nilsson (see the Notes to Section X.2). These results were further generalized by B. Hellwig, "Ein Kriterium für die Selbstadjungiertheit elliptischer Differentialoperatoren in $\mathbb{R}^n$," *Math. Z.* **86** (1964), 255–262 and "A criterion for self-adjointness of singular elliptic differential operators," *J. Math. Anal. Appl.* **26** (1969), 279–291. In particular, these papers contain a multi-dimensional version of Theorem X.8.

The second Corollary to Theorem X.38 is proven by alternative methods in H. Kalf, "Self-adjointness for strongly singular potentials with a $-|x|^2$ fall-off at infinity," *Math. Z.* **133** (1973), 249–255.

For Dirac operators, there is no restriction on how quickly V can grow at infinity. P. Chernoff in "Essential Self-Adjointness of Powers of Generators of Hyperbolic Equations," *J. Func. Anal.* **12** (1973), 401–414, remarked that this is intuitively correct since the relativistic bound $|v| < c$ prevents finite travel time to infinity. For strong results on the self-adjointness of Dirac operators, the reader can consult W. D. Evans, "On the Unique Self-Adjoint Extension of the Dirac Operator and the Existence of the Green Matrix," *Proc. London Math. Soc.* **20** (3) (1970), 537–557, and U.-W. Schmincke, "Essential Self-Adjointness of Dirac Operators with Strongly Singular Potentials," *Math. Z.* **126** (1972), 71–81.

Section X.6 Analytic vectors first appeared in the context of group representations in the work of Harish-Chandra, "Representations of a semi-simple Lie group on a Banach space, I," *Trans. Amer. Math. Soc.* **75** (1953), 185–243, and P. Cartier and J. Dixmier, "Vecteurs analytiques dans les représentations de groupes de Lie," *Amer. J. Math.* **80** (1958), 131–145. Their use in the study of a single operator was emphasized and developed by E. Nelson in "Analytic Vectors," *Ann. Math.* **70** (1959), 572–615. Given a continuous unitary representation $U(\cdot)$ of a Lie group G on a Hilbert space $\mathscr{H}$, Gårding had previously shown how to construct a common dense invariant domain for the generators of one-parameter subgroups of $U(G)$, i.e., for the representation of the Lie algebra g of G. In his paper, Nelson showed how to construct a common, dense, invariant domain of essential self-adjointness for all the generators by finding a domain that contained a dense set of analytic vectors for all the generators. Nelson also proved that if a Lie algebra is represented by symmetric operators on a dense invariant domain, then, if the domain contains a dense set of analytic vectors, the representation of the Lie algebra arises by differentiating a unique representation of the corresponding Lie group. These results have been extended; see, for example, J. Simon, "On the integrability of representations of finite-dimensional real Lie algebras," *Comm. Math. Phys.* **28** (1972), 39–46.

The generalization of Nelson's result given in Theorem X.40 is due to A. Nussbaum, "A note on quasi-analytic vectors," *Studia Math.* **33** (1969), 305–310. The simple proof outlined in Problem 42 originally appeared in B. Simon, "The theory of semi-analytic vectors: a new proof of a theorem of Masson and McClary," *Indiana Univ. Math. J.* **20** (1971) 1145–1151.

Nussbaum's lemma appears in "Quasi-analytic vectors," *Ark. Mat.* **6** (1965) 179–191. Nussbaum also introduced a generalization of the notion of analytic vectors. A vector $\varphi \in C^\infty(A)$ is called **quasi-analytic** if

$$\sum_{n=0}^{\infty} \|A^n\varphi\|^{-1/n} = \infty$$

An analytic vector is quasi-analytic, but the converse is not necessarily true. Nussbaum proves that a closed symmetric operator whose domain contains a dense set of quasi-analytic vectors is self-adjoint. Nussbaum also proves (in his *Studia Math.* paper) that a semibounded closed symmetric operator with a dense set of vectors satisfying

$$\sum_{n=1}^{\infty} \|A^n\varphi\|^{-1/2n} = \infty$$

is self-adjoint. Such vectors are called **Stieltjes vectors.** This result was obtained independently by D. Masson and W. McClary, "Classes of C^∞-vectors and essential self-adjointness," *J. Functional Analysis* **10** (1972) 19–32. Both the Nussbaum and the Masson–McClary papers use techniques from the moment problem. Essentially, they turn around the argument in Examples 4 and 6 and use classical results on the moment problem to prove that certain vectors are vectors of uniqueness. A critical result linking the two notions is in Nussbaum's *Arkiv* paper: $\varphi \in C^\infty(A)$ is a vector of uniqueness if and only if the Hamburger moment problem for $a_n = (\varphi, A^n\varphi)$ has a unique solution. The relationship between self-adjointness and the moment problem goes back at least as far as Stone's classic *Linear Transformations in Hilbert Space and Their Applications to Analysis*, Amer. Math. Soc. Colloquium Publication XV, New York (1932). Two general references for the moment problem are: J. Shohat and J. D. Tamarkin, *The Problem of Moments*, Amer. Math. Soc., New York, 1943, and Ya. V. Vorobyev, *Method of Moments in Applied Mathematics*, Gordon and Breach, New York, 1965.

Section X.7 Fock space was introduced by V. Fock in his paper "Konfigurationsraum und zweite Quantelung," *Z. Phys.* **75** (1932), 622–647. The first proof of the self-adjointness of the fields on Fock space was given by J. Cook: "The mathematics of second quantization," *Trans. Amer. Math. Soc.* **74** (1953), 222–245. Cook proved directly that $\varphi(f) \pm i$ and $\pi(f) \pm i$ have dense ranges on F_0.

The abstract structure of free fields was extensively studied in the 1950's by K. Friedrichs, *Mathematical Aspects of the Quantum Theory of Fields*, Wiley (Interscience), 1953, and by I. Segal in a series of papers; see especially "Tensor Algebras over Hilbert spaces, I," *Trans. Amer. Math. Soc.* **81** (1956), 106–134, where Q space was introduced. This led Segal to study the connection between the free field and probability theory and, in particular, he found a connection between abstract Fock spaces and Wiener path integrals.

For a discussion of the Wightman axioms, see Section IX.8 and the notes to that section. Wick ordering was introduced in G.-C. Wick: "The Evaluation of the Collision Matrix," *Phys. Rev.* **80** (1950), 267–272. General results on Wick ordered free fields may be found in L. Gårding and A. Wightman: "Fields as operator-valued distributions in relativistic quantum field theory," *Ann. Phys.* **16** (1961), 158–176.

Wick also emphasized the combinatorial structure of the vacuum expectation values of the free field. In particular, one has the following formulas:

$$(\Omega_0, \varphi(x_1) \cdots \varphi(x_n)\Omega_0) = 0 \qquad \text{if} \quad n \text{ is odd}$$

$$(\Omega_0, \varphi(x_1) \cdots \varphi(x_{2n})\Omega_0) = \sum_{\substack{i_1 < \cdots < i_n \\ i_k < j_k \\ i_1, \ldots, j_n \text{ distinct}}} (\Omega_0, \varphi(x_{i_1})\varphi(x_{j_1})\Omega_0) \cdots (\Omega_0, \varphi(x_{i_n})\varphi(x_{j_n})\Omega_0) \tag{X.162}$$

This complicated expression is a sum over all distinct ways of writing $\{1, \ldots, 2N\}$ as N pairs. (X.162) is one of a number of formulas that usually go under the name "Wick's theorem." Many of these formulas are well organized in a book by E. Caianiello, *Combinatorics and Renormalization in Quantum Field Theory*, Addison-Wesley, Reading, Massachusetts, 1973. (X.162) says that *for the free field* one can compute the Wightman distributions knowing only the two point function. There is a large class of models for which this is true: Let ρ be any polynomially bounded measure on $[0, \infty)$. Define

$$(\Omega_0, \varphi(x)\varphi(y)\Omega_0) = \int \Delta_+(x - y, m^2)\, d\rho(m^2)$$

and let the n-point distribution be given by (X.162). It can be shown that these distributions are the Wightman distributions of a unique quantum field theory satisfying the Wightman axioms. It is called the "generalized free field with spectral weight ρ." Like the free field, these theories are trivial in that the scattering matrix is the identity (when it exists). The generalized free field was introduced by W. Greenberg in "Generalized free fields and models of local field theory," *Ann. Phys.* **16** (1961), 158–176.

Number operator estimates of the kind found in Theorem X.44 were first used systematically by J. Glimm in "Yukawa coupling of quantum fields in two dimensions," *Comm. Math. Phys.* **5** (1967), 343–386. A thorough discussion of these estimates can be found in the lectures by J. Glimm and A. Jaffe "Some quantum field theory models" in *Statistical Mechanics and Quantum Field Theory* (Les Houches, 1970), ed. by C. deWitt and R. Stora, Gordon and Breach, New York, 1971.

We continue the study of the $(\varphi^4)_2$ model in Section X.9 and Chapter XIX where a detailed history will be given. L^p properties of the spatially cut-off interaction were first emphasized by E. Nelson, "A quartic interaction in two dimensions," in *Mathematical Theory of Elementary Particles* (R. Goodman and I. Segal, eds.), MIT Press, Cambridge, Massachusetts, 1966, who discovered the fact that $e^{-tV} \in L^1$. A detailed proof can be found in the Glimm–Jaffe lectures quoted above. For properties of the $(\varphi^4)_3$ interaction see J. Glimm and A. Jaffe, "Positivity of the $(\phi^4)_3$-Hamiltonian," *Fortschr. Physik* **21** (1973), 327–376, and the references therein.

The idea that Euclidean invariance is deeply connected with questions of inequivalence of representations of the CCR—an idea which is basic to our proof of Theorem X.46—is part of a complex of ideas generally called "Haag's theorem" after the discoveries of R. Haag in "On Quantum Field Theories," *Danske Vid. Selsk. Mat.-Fys. Medd.* **29** 12 (1955). The use of translation invariance suggests that the inequivalence of representations for different masses is "at infinity." This is true in the following sense: Given any bounded region B in $\mathbb{R}^3$ and free fields $\{\varphi_{m_1}, \pi_{m_1}\}$, $\{\varphi_{m_2}, \pi_{m_2}\}$ on $\mathscr{H}_1$ and $\mathscr{H}_2$, there is a unitary map U_B: $\mathscr{H}_1 \to \mathscr{H}_2$ so that $U_B \varphi_{m_1}(f) U_B^{-1} = \varphi_{m_2}(f)$ and $U_B \pi_{m_1}(f) U_B^{-1} = \pi_{m_2}(f)$ if supp $f \subset B$. This "local equivalence" appears again in Chapter XIX, both in our study of the free field algebras and in our discussion of the "local Fock property" of the $(\varphi^4)_2$ model.

Our construction of Q space is basis dependent in that it depended on the choice $\{f_n\}_{n=1}^{\infty}$. What is independent of the choice of basis is the algebra of measurable sets (modulo sets of measure zero) and the measure on these sets. There are many other "realizations" of Q space where the "points" differ, but the algebra of measurable sets and the measure are the same.

L. Gårding and A. S. Wightman classified all the representations of the relations (X.95) in "Representations of the canonical commutation relations," *Proc. Nat. Acad. Sci. U.S.A.* **40** (1954), 622–626. It is possible that von Neumann knew of the existence of inequivalent representations as early as 1938 since one can use his theory of infinite tensor products ("On Infinite Tensor Products," *Compositio Math.* **6** (1939), 1–77) to construct easily uncountably many inequivalent representations: see L. Streit: "Test function spaces for direct product representations," *Comm. Math. Phys.* **4** (1967), 22–31. The self-adjointness of the canonical fields of (X.95) in arbitrary representations was proven by M. Reed, "A Gårding domain for quantum fields," *Comm. Math. Phys.* **14** (1969), 336–346. Reed showed that for any representation in the Gårding–Wightman classification, there is a Banach space B of test functions (B depends on the representation) so that $\varphi(f)$ and $\pi(f)$ are self-adjoint for $f \in B$.

A classification of representations of the CCR in continuous form (X.94) can be found in several places; see, e.g., I. M. Gel'fand and N. Vilenkin, *Generalized Functions IV*, Academic Press, New York, 1964, p. 370. Reed's theorem has been extended to the continuous CCR by G. Hergerfeldt, "Gårding domains and analytic vectors for quantum fields," *J. Math. Phys.* **13** (1972), 821–827. His theorem is quoted on page 232.

Section X.8 The study of semigroups of linear transformations has its origin in M. Stone's paper on unitary groups in Hilbert space: "Linear transformations in Hilbert space III," *Proc. Nat. Acad. Sci. U.S.A.* **16** (1930), 172–175. The Hille–Yosida theorem for the case of contraction semigroups (Theorem X.47a) was proven independently by E. Hille: *Functional analysis and semi-groups*, Amer. Math. Soc. Colloquium Publication, **31**, 1948, New York, and "On the generation of semi-groups and the theory of conjugate functions," *Kungl. Fys. Sälls. I Lund Förhand.* **21** (1952), 1–13, and by K. Yosida: "On the differentiability and representation of one-parameter semi-groups of linear operators," *J. Math. Soc. Japan* **1** (1948), 15–21. The generalization (Theorem X.47b) appeared shortly thereafter in W. Feller, "On the generation of unbounded semi-groups of bounded linear operators," *Ann. Math.* **58** (1953), 166–174, I. Miyadera: "Generation of a strongly continuous semi-group of operators," *Tôhoku Math. J.* **4** (1952), 109–114, and R. S. Phillips: "Perturbation theory for semi-groups

of linear operators," *Trans. Amer. Math. Soc.* 74 (1953), 343–369. Theorem X.47b is usually called the Hille–Yosida–Phillips theorem.

There are various other conditions besides strong continuity on $[0, \infty)$ which can be put on $T(t)$. For example, one can require:

(i) $T(t)$ is strongly measurable
(ii) $T(t)$ converges strongly to I as $t \downarrow 0$
(iiia) $\int_0^1 \|T(t)\|\, dt < \infty$
(iiib) $\lim_{\lambda\to\infty} \lambda \int_0^\infty e^{-\lambda t} T(t)\varphi = \varphi$ for all $\varphi \in X$.

It can be shown that (i) and (ii) together imply strong continuity on $[0, \infty)$. Another possible set of hypotheses is (i) and (iii). In this case $\|T(t)\|$ can be unbounded as $t \to 0$. As in the case of strong continuity, there is a theorem classifying the generators of such semi-groups. A detailed study of various continuity conditions as $t \to 0$ and the corresponding classification of generators may be found in E. Hille and R. S. Phillips: *Functional Analysis and Semi-groups*, Amer. Math. Soc. Colloquium Publication, 1957, New York.

The term "accretive" originally appeared in K. Friedrichs, "Symmetric positive linear differential equations," *Comm. Pure Appl. Math.* **11** (1958), 333–418. The study of such operators was essentially initiated by R. S. Phillips in his paper quoted above. For a semigroup e^{-tA}, Phillips calls $-A$ (rather than A) the generator. Therefore in the Hilbert space case, his generators satisfy $\mathrm{Re}(\varphi, A\varphi) \leq 0$ (rather than $\mathrm{Re}(\varphi, A\varphi) \geq 0$). He calls such operators "dissipative." The theory of dissipative operators on Banach spaces is due to G. Lumer and R. S. Phillips: "Dissipative operators in a Banach space," *Pacific J. Math.* **11** (1961), 679–698. This paper contains a counterexample which shows that a maximal accretive operator need not generate a semigroup in the Banach space case. The fact that maximal accretive operators do generate semigroups in the Hilbert space case appeared in R. S. Phillips, "Dissipative operators and hyperbolic systems of partial differential equations," *Trans. Amer. Math. Soc.* **90** (1959), 193–254.

An example of a bounded semigroup which is not a contraction semigroup is

$$\begin{pmatrix} \cos\theta & 2\sin\theta \\ -\frac{1}{2}\sin\theta & \cos\theta \end{pmatrix}$$

on $\mathbb{R}^2$. Infinite dimensional bounded semigroups which are not contractions enter in the scattering theory associated to the linearized Boltzmann equation; see Chapter XII.

In the finite-dimensional case, every semigroup obeys $\lim_{t\downarrow 0} \|T(t)\| = 1$. However, in the infinite-dimensional case this need not be true (see Example 5). When this norm condition fails there is no simple characterization of the generator directly in terms of $\ell(A\varphi)$.

Theorem X.50 is due to Gustafson: "A perturbation lemma," *Bull. Amer. Math. Soc.* **72** (1966), 334–338. The proof we give (for $a < \frac{1}{2}$) is due to E. Nelson: "Feynman integrals and the Schrödinger equation," *J. Math. Phys.* **5** (1964), 332–343, though some of the ideas already appeared in H. Trotter: "On the product of semi-groups of operators," *Proc. Amer. Math. Soc.* **10** (1959), 545–551. Nelson's and Trotter's papers also contain their proofs of the general Trotter product formula. A simplification and generalization of Trotter's theorem appears in P. R. Chernoff, "Semigroup product formulas and addition of unbounded operators," *Bull. Amer. Math. Soc.* **76** (1970), 395. The corollary to Theorem X.50 has been extended to the case where $a = 1$ in the case that X is a reflexive Banach space. This generalizes Wüst's theorem and is proven by similar methods in P. R. Chernoff, "Perturbations of dissipative operators of relative bound one," *Proc. Amer. Math. Soc.* **33** (1972), 72–74.

Theorem X.52 is due to E. Hille and R. S. Phillips (their book cited above) and K. Yosida: "On the differentiability of semi-groups of linear operators," *Proc. Japan Acad.* **34** (1958), 337–340. The proof of holomorphicity in Theorem X.55 follows E. Stein: *Topics in Harmonic Analysis*, Ann. Math. Studies, Princeton Univ. Press, Princeton, New Jersey. Dunford–Taylor type formulas for holomorphic semigroups are very important for they allow the computation of various quantities by the Cauchy integral formula.

A spectral mapping theorem for semigroups is discussed in Section XIII.8.

The connection between partial differential equations and semigroup theory goes back to J. Hadamard who noticed that the solution of the Cauchy problem has the semigroup property with respect to t: "Sur un problème mixte aux dérivées partielles," *Bull. Soc. Math. France* **31** (1903), 208–224, and "Principe de Huygens et prolongement analytique," *Bull. Soc. Math. France* **52** (1924), 241–278. But semigroup theory was not applied systematically to partial differential equations until Hille and Yosida developed the analytical tools in the late 1940's. The examples given in the text suggest that one should be able to apply semigroup theory to general second-order parabolic partial differential equations, i.e., equations of the form $\partial u(x, t)/\partial t = Au(x, t)$ where

$$A\varphi = \sum_{i,j} \frac{\partial}{\partial x_i} a_{ij}(x) \frac{\partial}{\partial x_j} \varphi(x) + \sum_i \frac{\partial}{\partial x_i} b_i(x)\varphi(x) + c(x)\varphi(x)$$

is elliptic in an appropriate sense. This is in fact true but the applications are not easy for several reasons. First, in the case of nonconstant coefficients or a bounded domain, the Fourier transform is no longer available, so one must prove that A satisfies the conditions of Theorems X.47, X.52 by a priori estimates (like Gårding's inequality) and the Hahn–Banach theorem (to show $\mathrm{Ran}(A + \lambda)$ is dense). The situation is further complicated since A (restricted to a nice domain of functions) will have many closed extensions and one must choose the "right one" as the generator. Finally, one uses a generalization of Weyl's lemma (see Section IX.6) to prove regularity. Among the fundamental papers applying semigroup techniques to parabolic equations are: W. Feller, "The parabolic differential equations and the associated semigroups of transformations," *Ann. Math.* **55** (1952), 468–519; P. Lax and A. Milgram, "Parabolic equations" in *Contributions to the Theory of Partial Differential Equations*, Princeton Univ. Press, Princeton, New Jersey, 1954; P. Lax and R. S. Phillips, "Local boundary conditions of dissipative systems of linear partial differential operators," *Comm. Pure Appl. Math.* **13** (1960), 427–455; R. S. Phillips, "On the integration of the diffusion equation with boundaries," *Trans. Amer. Math. Soc.* **98** (1961), 62–84; K. Yosida, "An abstract analyticity in time for solutions of a diffusion equation," *Proc. Japan Acad.* **35** (1959), 109–113. Certain kinds of parabolic equations which are nonlinear or where A depends on t (called evolution equations) can also be handled with semigroup methods; see A. Friedman, *Partial Differential Equations*, Holt, New York, 1969. There is an extensive literature on semigroups of nonlinear operators; see Section X.13 and its notes.

It was noticed by E. Hille in *Functional Analysis and Semi-groups*, Amer. Math. Soc. Colloquium Publication **31**, 1949, New York, that semigroup theory could also be applied to hyperbolic equations. For the wave equation with constant coefficients, the method is outlined in Problem 60. In a nonlinear context, this idea is exploited in Section X.13. For the semigroup approach to a broad class of hyperbolic problems, see R. S. Phillips, "Dissipative operators and hyperbolic systems of partial differential equations," *Trans. Amer. Math. Soc.* **90** (1959), 193–254.

The second main area of application of semigroup techniques is in probability theory. The connection between the heat equation and probability theory was discovered by A. Einstein, "Über die von der molecularkinetischen Theorie der Wärme geforderte Bewegung von in ruhenden Flüssigkeiten suspendierten Teilchen," *Ann. Physik* **17** (1905), 549–560. But it was not until 1952 that Feller initiated a systematic study of semigroups in probability theory in

the paper quoted above. The theory was developed in G. Hunt, "Markov processes and potentials, I," *Illinois J. Math.* **1** (1957), 44–93; II, **1** (1957), 316–369; III, **2** (1958), 151–213; and "Semigroups of measures on Lie groups," *Trans. Amer. Math. Soc.* **81** (1956), 264–293. For a description of these applications, see the probability theory books quoted in the notes to Section X.11.

We mentioned at the beginning of the section that accretive operators generalize to Banach spaces many important properties of self-adjoint operators. The main tool that does not generalize to all accretive operators is the spectral resolution. A class of "spectral operators" which do admit a kind of spectral resolution was introduced in N. Dunford: "Spectral operators," *Pacific J. Math.* **4** (1954), 321–354. An exhaustive study of such operators may be found in N. Dunford and J. Schwartz, *Linear Operators, III, Spectral Operators*, Wiley (Interscience), New York, 1971.

Section X.9 The theory of hypercontractive semigroups is an abstraction of certain developments in constructive quantum field theory. The germinal ideas appeared in E. Nelson, "A quartic interaction in two dimensions," in *Mathematical Theory of Elementary Particles*, pp. 69–73, (R. Goodman and I. Segal, eds.) M.I.T. Press, Cambridge, Massachusetts, 1966. Nelson isolated those properties of Hermite operators (Example 1) which we now call hypercontractive and used them together with the theory of Feynman path integrals to prove that certain field theoretic Hamiltonians are bounded below. This work was clarified and extended by J. Glimm, "Boson fields with nonlinear self-interaction in two dimensions," *Comm. Math. Phys.* **8** (1968), 12–25. In particular, Glimm introduced the use of the Riesz–Thorin theorem. Nelson's ideas played a role in the first proof of self-adjointness of the spatially cutoff $(\varphi^4)_2$ Hamiltonian $H_0 + H_I(g)$ by Glimm and Jaffe, "A $\lambda\varphi^4$ quantum field theory without cutoffs," *Phys. Rev.* **176** (1968), 1945–1951. Glimm and Jaffe also used graph convergence (see Section X.10) and Feynman path integrals in their proof. The basic ideas of hypercontractivity emerged from the independent work of L. Rosen and I. Segal. Rosen in "A $\lambda\varphi^{2n}$ theory without cutoffs," *Comm. Math. Phys.* **16** (1970), 157–183, gave a proof of essential self-adjointness of $P(\varphi)_2$ Hamiltonians which used hypercontractivity and Feynman path integrals. While it was not fully realized at the time, Rosen's proof depended on little more than L^p techniques and contained all the main ideas of the abstract $H_0 + V$ theory. Segal in "Notes towards the construction of nonlinear relativistic quantum fields, III: Properties of the C^*-dynamics for a certain class of interactions," *Bull. Amer. Math. Soc.* **75** (1969), 1390–1395, showed that it was possible to replace completely the use of Feynman path integrals with the Trotter product formula and that hypercontractivity could be used to provide a self-adjoint operator H which was formally $H_0 + V$. In addition, what we have called Segal's lemma appeared and it was used to simplify the earlier lower boundedness proofs of Nelson and Glimm. Segal also clarified a point in the earlier proofs concerning the question of whether the tensor product of contractions from L^2 to L^4 is necessarily a contraction. An alternative discussion of this fact can be found in the Les Houches lectures of Glimm and Jaffe quoted in the notes to Section X.7. In his fuller paper, "Construction of nonlinear quantum processes, I," *Ann. Math.* **92** (1970) 462–481, Segal supplemented this with a proof of the essential self-adjointness of $H_0 + V$ on $D(H_0) \cap D(V)$. That essential self-adjointness holds on $C^\infty(H_0) \cap D(V)$ was proven in an appendix to B. Simon, "Essential Self-Adjointness of Schrödinger Operators with Positive Potentials," *Math. Ann.* **201** (1973), 211–220. For the special case of the $(\varphi^4)_2$ Hamiltonian, this had already been proven by very different means in the Glimm and Jaffe paper mentioned above. For the case of the $(\varphi^{2n})_2$ Hamiltonian it had been proven in L. Rosen, "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457.

The theory of hypercontractive semigroups has been extended and clarified by a variety of authors. B. Simon and R. Höegh-Krohn in "Hypercontractive semi-groups and two-dimensional self-coupled Bose fields," *J. Functional Analysis* **9** (1972), 121–180, reviewed the basic theory and its use in the $P(\varphi)_2$ model, extended it in certain directions and, coined the term "hypercontractive." The special case of contractive semigroups was first emphasized for its own sake and applied in R. Höegh-Krohn, "A general class of quantum field theories without cutoff in two space-time dimensions," *Comm. Math. Phys.* **21** (1971), 244–255. Extensions to still more abstract settings can be found in I. Segal, "Construction of nonlinear local quantum processes, II," *Invent. Math.* **14** (1971), 211–241, W. Faris, "Quadratic forms and essential self-adjointness," *Helv. Phys. Acta* **45** (1972), 1074–1088 and W. Faris, "Essential self-adjointness of operators in ordered Hilbert space," *Comm. Math. Phys.* **30** (1973), 23–34. In his *Helv. Phys. Acta* paper, Faris gives an interesting "explanation" in terms of quadratic forms of why hypercontractivity should imply self-adjointness. Further applications of the hypercontractivity method in constructive quantum field theory appear in the paper of Höegh-Krohn quoted above and in A. Klein, "Self-adjointness of the locally correct generator of Lorentz transformations for $P(\varphi)_2$," in *Mathematics of Contemporary Physics* (R. Streater, ed.), Academic Press, New York, 1973, and "Quadratic expressions in a free Boson field," *Trans. Amer. Math. Soc.* **181** (1973), 439–456. Extensions of some of the ideas to fermion theories appear in L. Gross, "Existence and uniqueness of physical ground states," *J. Functional Analysis* **10** (1972), 52–109.

The simple proof of the hypercontractivity of Hermite operators which we give (Example 1) is due to E. Nelson, "The free Markov field," *J. Functional Analysis* **12** (1973), 211–227. Earlier proofs of hypercontractivity obtain Theorem X.61 in the infinite-dimensional case by a two-step process from the case of a one-dimensional one particle space. First one shows that knowing that e^{-tH_0} is bounded from L^2 to L^4 for some t and that H_0 has a gap in its spectrum above zero, one can conclude that e^{-TH_0} is actually a contraction from L^2 to L^4 for T sufficiently large. The infinite-dimensional case is then controlled by discussing tensor products of contractions from L^2 to L^4. The proof of Nelson in the one-dimensional case that we give in the text generalizes to arbitrary dimensions and so avoids the two step process. In fact, one can turn one of the steps around and prove directly that the map e^{-TH_0} is a contraction from L^2 to L^4 for suitable T. For further discussion of these points, the reader should consult Section I.5 of Simon's lectures referred to in the Notes to Section X.11.

In the above paper, Nelson also proves the following best possible bounds: Let $\mathscr{H}$ be a complex Hilbert space with distinguished complex conjugation. Let A be a bounded operator on $\mathscr{H}$ commuting with the conjugation. Let Q be the Q-space built over the Fock space on $\mathscr{H}$ according to the construction in Section 7. Then $\Gamma(A)$ is a bounded operator from $L^p(Q)$ to $L^q(Q)$ $(p \leq q)$ if and only if $\|A\| \leq \sqrt{(p-1)/(q-1)}$ and in that case it is a contraction. An alternative proof of this theorem appears in L. Gross, "Logarithmic Sobolev inequalities," *Amer. J. Math.* (to appear).

Segal's lemma can be viewed as a special case of a more general result. Let $\|\cdot\|_\infty$ denote the operator norm of $\mathscr{L}(\mathscr{H})$, then Segal's lemma says that

$$\|e^{(A+B)}\|_\infty \leq \|e^{A/2}e^{B}e^{A/2}\|_\infty$$

There is an inequality of S. Golden, "Lower bounds for the Helmholtz function," *Phys. Rev.* **137B** (1965), 1127–1128, and C. Thompson, "Inequality with applications in statistical mechanics," *J. Math. Phys.* **6** (1965), 1812–1813, which says that for A and B self-adjoint

$$\mathrm{Tr}(e^{A+B}) \leq \mathrm{Tr}(e^{A}e^{B})$$

or equivalently that

$$\|e^{A+B}\|_1 \leq \|e^{A/2}e^{B}e^{A/2}\|_1$$

It is also possible to prove that

$$\|e^{A+B}\|_p \leq \|e^{A/2}e^{B}e^{A/2}\|_p$$

for any p. The Golden–Thompson inequality is further discussed in A. Lenard, "Generalization of the Golden–Thompson inequality," *Indiana Univ. J. Math.* **21** (1971), 457–468, M. B. Ruskai, "Inequalities for Traces on von Neumann Algebras," *Comm. Math. Phys.* **26** (1972), 280–289, and C. Thompson, "Inequalities and partial orders on matrix spaces," *Indiana Univ. J. Math.* **21** (1971), 469–480.

Section X.10 The basic ideas and theorems in Section 10 are due to J. Glimm and A. Jaffe: "Singular perturbations of self-adjoint operators," *Comm. Pure Appl. Math.* **22** (1969), 401–414. Glimm and Jaffe used their results to give the first proof of the self-adjointness of the spatially cut-off $(\varphi^4)_2$ Hamiltonian (see the notes to Section X.7). The existence of the spatially cut-off Hamiltonian for the Yukawa theory was proven in two papers: Resolvent convergence was established in J. Glimm and A. Jaffe, "Self-adjointness for the Yukawa$_2$ Hamiltonian," *Ann. Physics.* **60** (1970), 321–383. That the sequence $\{H(g, n)\}_{n=1}^{\infty}$ is bounded below and densely bounded had already been proven by Glimm in "Yukawa coupling of quantum fields in two dimensions, I," *Comm. Math. Phys.* **5** (1967), 343–386. For a general discussion see the Les Houches lectures referred to in the notes to Section X.7.

The techniques used in the example can be extended to the case of the x^{2n} oscillator by using ideas from L. Rosen: "The $(\varphi^{2n})_2$ quantum field theory: Higher order estimates," *Comm. Pure Appl. Math.* **24** (1971), 417–457.

Section X.11 The first work on Wiener measure appeared in N. Wiener's paper, "Differential space," *J. Math. Phys.* **2** (1923). Wiener introduced his measure in order to make rigorous the work of Einstein and Smoluchowski on Brownian motion. The reader can find a discussion of the history of the study of Brownian motion in E. Nelson, *Dynamical Theories of Brownian Motion*, Princeton Univ. Press, Princeton, New Jersey, 1967. The construction of Wiener measure which we give is due to Nelson in "Feynman Integrals and the Schrödinger Equation," *J. Math. Phys.* **5** (1964), 332–343. The argument in Problem 64 showing that it is impossible to construct an imaginary time Feynman path (complex) measure is due to R. Cameron, "The Ilstow and Feynman Integrals," *J. Anal. Math.* **10** (1962/63), 287–361. The reader should be wary of an erroneous construction in I. Gel'fand and A. Yaglom, "Integration in function spaces and its applications to quantum physics," *J. Math. Phys.* **1** (1960), 48–69.

There is a large textbook literature on Wiener measure from a probabilistic point of view: J. Doob, *Stochastic Processes*, Wiley, New York, 1953; E. Dynkin, *Markov Processes*, Vol. I, II, Springer-Verlag, Berlin, 1965; T. Hida, *Stationary Stochastic Processes*, Princeton Univ. Press, Princeton, New Jersey, 1970; K. Itô and H. McKean, *Diffusion Processes and their Sample Paths*, Springer-Verlag, Berlin, 1965; M. Kac, *Probability and Related Topics in the Physical Sciences*, Wiley (Interscience), New York, 1959. The reader who is interested in but ignorant of the probabilistic background might profit from M. Reed, "Functional Analysis and Probability Theory," in *Constructive Quantum Field Theory* (G. Velo and A. Wightman, eds.), *Springer Lecture Notes in Physics* **25**, 1973, 1–41. A wealth of detailed information about regularity properties of Wiener measure, and in particular Theorem X.67, can be found in the Itô–McKean book.

Some of the probability literature, especially the older literature, contains technical complications which do not appear in our discussion. This is because some authors construct Wiener measure in such a way that, when translated to our terminology, it is only a Baire measure. Some nice subsets of Ω, such as Ω_α, are Borel sets but not Baire sets. The idea of avoiding some technical complications by realizing Ω as a compact product space and using regular Borel measures is due to E. Nelson, "Regular Probability Measures on Function Space," *Ann. Math.* **67** (1954), 630–643. Unfortunately, Nelson's method does not remove all measurability problems, since in further developments some non-Borel sets, such as the paths that are continuous from the right, are important.

Feynman's idea of expressing the Schrödinger dynamics in terms of a sum over histories appeared in his Princeton thesis (1942) and in R. Feynman, "Space-time approach to non-relativistic quantum mechanics," *Rev. Modern Phys.* **20** (1948), 367–387. The reader can find a detailed exposition and further developments in R. Feynman and A. Hibbs, *Quantum Mechanics and Path Integrals*, McGraw-Hill, New York, 1965. The idea of continuing to imaginary time so that Wiener measure can be used and the Feynman–Kac formula appeared in M. Kac, "On some connections between probability theory and differential and integral equations," *Proceedings of the Second Berkeley Symposium on Mathematical Statistics and Probability*, Univ. of California Press, Berkeley, 1951, 189–215. Our proof of the Feynman–Kac formula is taken from E. Nelson's *J. Math. Phys.* paper quoted above.

Path integrals have played a major role in constructive quantum field theory, especially in the recent theory of Euclidean and Markov fields. Path integral methods were first advocated in constructive quantum field theory by E. Nelson in the first paper quoted in the notes to Section X.9 and in Euclidean quantum field theory by Nelson in "Quantum fields and Markov fields," in *Partial Differential Equations* (D. Spencer, ed.) *Symp. Pure Math.* **23**, Amer. Math. Soc., Providence, Rhode Island, 1973, pp. 211–219. The reader can find further discussion of these methods and their development in *Constructive Quantum Field Theory* (G. Velo and A. Wightman eds.), *Springer Lecture Notes in Physics* **25**, 1973, and in B. Simon, *The $P(\varphi)_2$ Euclidean (Quantum) Field Theory*, Princeton Univ. Press, Princeton, New Jersey, 1974.

Section X.12 The idea of using an expansion like the Dyson expansion to find a propagator $U(t, s)$ satisfying

$$\frac{d}{dt}U(t, s) = -iH(t)U(t, s), \qquad U(s, s) = I \tag{X.163}$$

is essentially the method of successive substitution developed in the nineteenth century to solve integral equations. (X.163) is formally equivalent to the integral equation

$$U(t, s) = I - i\int_s^t H(r)U(r, s)\,dr$$

The Dyson expansion results from repeatedly substituting this expression for $U(t, s)$ under the integral. Dyson used the expansion to give a perturbation theoretic description of quantum electrodynamics in "The radiation theories of Tomonaga, Schwinger, and Feynman," *Phys. Rev.* **75** (1949), 486–502, and "The S-matrix in quantum electrodynamics," *Phys. Rev.* **75** (1949), 1736–1755.

T. Kato in "Integration of the equation of evolution in a Banach space," *J. Math. Soc. Japan* **5** (1953), 208–234, was the first to find general conditions for the solution of the evolution equation $d\varphi(t)/dt = A(t)\varphi(t)$ where $A(\cdot)$ is an unbounded-operator valued function. Since one of the main applications of this theory is in partial differential equations, there were

many special results before that. In proving Theorem X.70 we have followed closely the proof due to K. Yosida, *Functional Analysis*, 2nd ed. Springer-Verlag, Berlin, 1968, pp. 224–230. For more general results, see T. Kato, "Linear evolution equations of hyperbolic type," *J. Fac. Sci. Univ. Tokyo Sect. I, A Math.* **17** (1970), 241–258.

See B. Simon, *Quantum Mechanics for Hamiltonians defined as quadratic forms*, Princeton Univ. Press, Princeton, New Jersey, 1971, for a discussion of time-dependent form results and, in particular, extensions of Theorem X.71 to the Rollnik class.

The idea of using the Hilbert space $L^2(\mathbb{R}; \mathscr{H})$ to change time-dependent quantum Hamiltonians to time-independent ones is due to J. Howland, "Stationary scattering theory for time-dependent Hamiltonians," *Math. Ann.* **207** (1974), 315–335. One nice application of Howland's idea is to scattering theory. Let $U(t, s)$ and $U_0(t, s)$ be two unitary propagators on $\mathscr{H}$ and let $\hat{U}(\sigma)$ and $\hat{U}_0(\sigma)$ be the corresponding strongly continuous one-parameter groups on $L^2(\mathbb{R}; \mathscr{H})$. Then one can show that the wave operators for the time-dependent theory on $\mathscr{H}$ exist if and only if the usual wave operators

$$W_\pm = s - \lim_{\sigma \to \infty} \hat{U}_0(-\sigma)\hat{U}(\sigma)$$

exist on $L^2(\mathbb{R}; \mathscr{H})$. Therefore one can prove the existence of wave operators in certain theories with time-dependent Hamiltonians by reformulating as above and using the usual methods for the case where the Hamiltonians do not depend on time. For proofs of these results and those mentioned in the text, see Howland's paper.

There is another method for constructing propagators which *formally* satisfy (X.163). Namely, suppose that $\mathscr{B}$ is a Banach space whose elements are unbounded-operator valued functions on some fixed compact subinterval of $\mathbb{R}$. Suppose that $\mathscr{B}$ contains a dense subset $\mathscr{B}_0$ so that whenever $f \in \mathscr{B}_0$, (X.163) has a strict solution with $H = H_0 + f(t)$ for some fixed operator H_0. Let $U(t, s; f)$ denote the corresponding propagator. If $U(t, s; \cdot)$ is uniformly continuous on $\mathscr{B}_0$, then we can extend $U(t, s; \cdot)$ to $\mathscr{B}$ to obtain formal solutions of (X.163) for $f \in \mathscr{B}$. We will see an example of this in the appendix to Section XIII.6.

Section X.13 The original proof of the existence of global solutions of (X.138) ($m > 0$) is due to K. Jörgens, "Das Anfangswertproblem im Grossen für eine Klasse nichtlinearer Wellengleichungen," *Math. Z.* **77** (1961), 295–308. The abstract approach to such non-linear problems was developed in F. Browder, "On non-linear wave equations," *Math. Z.* **80** (1962), 249–264, and I. Segal, "Non-linear semi-groups," *Ann. Math.* **78** (1963), 339–364. A global existence theorem for the mass zero case was first proven in W. Strauss, "Decay and asymptotics for $\Box u = F(u)$," *J. Functional Analysis* **2** (1968), 409–457. The mass zero case can also be handled directly by the methods in Section X.13. The procedure is outlined in Problem 76. Similar techniques have also been applied to the coupled Maxwell–Dirac equations; see L. Gross, "The Cauchy problem for the coupled Maxwell and Dirac equations," *Comm. Pure Appl. Math.* **19** (1966), 1–15, and J. Chadam, "On the Cauchy problem for the coupled Maxwell–Dirac equations," *J. Math. Phys.* **13** (1972), 597–604; "Global solutions of the Cauchy problem for the (classical) coupled Maxwell–Dirac equations in one space dimension," *J. Functional Analysis* **13** (1973), 173–184.

The nonexistence of global solutions for certain nonlinear partial differential equations has been known for a long time; see, for example, J. Keller, "On solutions of non-linear wave equations," *Comm. Pure Appl. Math.* **10** (1957), 523–532. The example used at the end of the section was described to the authors by H. Levine. Generalizations of the example appear in his paper "Some non-existence and instability theorems for solutions of formally parabolic equations of the form $Pu_t = -Au + \tilde{F}(u)$," *Arch. Rational Mech. Anal.* **51** (1973), 371–386.

Let $\varphi(t) = \langle u(x, t), u_t(x, t) \rangle$ be the solution of the nonlinear Klein–Gordon problem described in the text and define M_t to be the mapping $M_t : \varphi(0) \to \varphi(t)$. Then M_t is a strongly continuous semigroup of bounded *nonlinear* operators. The question immediately arises whether the theory of strongly continuous semigroups of *linear* operators described in Section X.8 has a counterpart in the nonlinear case. In particular, do such nonlinear semigroups have unique infinitesimal generators? A large literature has grown about these questions. See, for example, T. Kato's article "Accretive operators and non-linear evolution equations in Banach spaces," pp. 138–161, in *Proc. Symp. Pure Math.* **18**, Part I, Amer. Math. Soc. 1970, (F. Browder, ed.) or M. Crandall's article "Semi-groups of nonlinear transformations in Banach spaces," pp. 157–171, in *Contributions to Nonlinear Functional Analysis* (E. Zarantonello, ed.), Academic Press, New York, 1971, and the references therein.

Section X.14 A fairly readable account of Hamiltonian mechanics (but with some mathematical errors) may be found in H. Goldstein, *Classical Mechanics*, Addison-Wesley, Reading, Massachusetts, 1950. A more sophisticated presentation is contained in R. Abraham, *Foundations of Mechanics*, Benjamin, New York, 1967.

The natural setting for classical mechanics is a symplectic manifold. A quadratic form q on a finite-dimensional real vector space is called **symplectic** if: (1) $q(v, w) = -q(w, v)$, (2) q is nondegenerate, i.e., $q(v, w) = 0$ for all w implies that $v = 0$. A **symplectic manifold** is a differential manifold M with a distinguished 2-form $\omega \in \Lambda^2(M)$ so that (1) $d\omega = 0$, (2) for each x, ω_x is a symplectic form on the tangent space $T_x(M)$. ω sets up a bijective map ω_*, of $T(M)$, the tangent bundle, to the cotangent bundle $T^*(M)$ by: $[\omega_*(X)](Y) = \omega(X, Y)$. Given $f, g \in C^\infty(M)$, their Poisson bracket is defined by $\{f, g\} = [\omega_*^{-1}(df)](g)$. Given a function H in $C^\infty(M)$, we define the associated Hamiltonian flow by $\dot{p}(t) = (Xp)(t)$ where X is the vector field $X = -\omega_*^{-1}(dH)$. There is a natural volume form defined by ω; namely $\wedge^n\omega \in \wedge^{2n}(M)$ if $2n = \dim(M)$. Liouville's theorem asserts that $\wedge^n\omega$ is left invariant by any Hamiltonian flow. The cotangent bundle of any manifold is a symplectic manifold in a natural way.

The L^2 version of Liouville's theorem is that L is skew symmetric. The idea of using Theorem VIII.11 to prove skew-adjointness of L can be found in W. Hunziker, "The S-matrix in classical mechanics," *Comm. Math. Phys.* **8** (1968), 282–299. The general idea of using existence theorems for first order systems to prove essential self-adjointness of differential operators is further exploited in P. Chernoff, "Essential self-adjointness of powers of generators of hyperbolic equations," *J. Functional Analysis* **12** (1973), 401–414. Chernoff uses the fact that if $U_t = e^{-iAt}$ leaves a dense set D invariant and $D \subset C^\infty(A)$, then A^n is essentially self-adjoint on D for any n. By an extra trick, this can be used to handle operators which do not appear to be squares of first order operators, e.g. $-\Delta$ on $L^2(\mathbb{R}^3)$. For let $\mathscr{H} = L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3; \mathbb{R}^3) \oplus L^2(\mathbb{R}^3; \mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ and let $d(f, \mathbf{g}, \mathbf{h}, k) = (0, \operatorname{grad} f, \operatorname{curl} \mathbf{g}, \operatorname{div} \mathbf{h})$ so that $d^*d(f, \mathbf{g}, \mathbf{h}, k) = (-\Delta f, \ldots)$ and $d^2 = 0$. Let $A = d + d^*$. Then A^2 restricted to the first summand is $-\Delta$. Of course, this is a hard way to control $-\Delta$ on $L^2(\mathbb{R}^3)$ but the method allows one to prove that the Laplace–Beltrami operator is essentially self-adjoint on $C^\infty(M)$ for a wide class of Riemannian manifolds. Chernoff's methods also work to prove:

Theorem If V is in $C^\infty(\mathbb{R}^3)$ and α, β are the usual Dirac matrices, then

$$H = -\alpha \cdot i\partial + \beta m + V$$

is essentially self-adjoint on $C^\infty(\mathbb{R}^3)$.

Unlike the Schrödinger operator case, there are no growth conditions on V. As Chernoff remarks, this should not be surprising since the relativistic bound on velocities prevents finite travel time to infinity.

If H has singularities such as Coulomb singularities, one cannot ask that global solutions for (X.153) exist for all initial conditions since collisions might take place. In the multiparticle case worse horrors can be imagined. Instead, one would like to prove global solutions exist for almost all initial conditions. This is known as **almost completeness**. Almost completeness can be proven for the two-body problem using angular momentum conservation, and it can be proven for the three-body problem by using results of K. Sundman, "Le problème des trois corps," *Acta Soc. Sci. Fenn.* **35** (1909), and G. D. Birkhoff, *Dynamical Systems*, Amer. Math. Soc. Colloq. Publ. **1**, *IX* (1927). Partial results toward the N-body problem can be found in H. Pollard and D. G. Saari, "Singularities of the N-Body Problem, I, II," *Arch. Rational Mech. Anal.* **30** (1968), 263–269; in *Inequalities*, II, ed. O. Shisha, Academic Press, New York, 1970, and in D. G. Saari, "Improbability of collisions in Newtonian gravitational systems," *Trans. Amer. Math. Soc.* **162** (1971), 267–271; erratum **168** (1972), 521.

Discussions of some of the more interesting mathematical problems in classical mechanics can be found in Abraham's book and in H. Pollard, *Mathematical Introduction to Celestial Mechanics*, Prentice-Hall, Englewood Cliffs, New Jersey, 1966; C. L. Siegel and J. K. Moser, *Lectures on Celestial Mechanics*, Springer-Verlag, Berlin, 1971, and S. Sternberg, *Celestial Mechanics*, Part I, II, Benjamin, New York, 1969.

Finally we should mention the beautiful work of Lanford on existence of solutions of Newton's equations for certain systems with infinitely many particles: O. E. Lanford, III, "The classical mechanics of one-dimensional systems of infinitely many particles, I, II," *Comm. Math. Phys.* **9** (1968), 176–191; **11** (1969), 257–292.

PROBLEMS

1. (a) Let A_n be symmetric on $\mathscr{H}_n$ and D be the set of vectors in $\bigoplus_{n=1}^{\infty} \mathscr{H}_n$ of the form $\psi = (\psi_1, \psi_2, \ldots)$ where $\psi_n \in D(A_n)$ and all but finitely many ψ_n are zero. Show that $A = \sum_{n=1}^{\infty} A_n$ is symmetric on D and that $n_+(A) = \sum_{n=1}^{\infty} n_+(A_n)$, $n_-(A) = \sum_{n=1}^{\infty} n_-(A_n)$.
   (b) Show that $i\,d/dx$ on $C_0^\infty(0, \infty)$ has deficiency indices $n_+ = 0$, $n_- = 1$. Show that $i\,d/dx$ on $C_0^\infty(-\infty, 0)$ has deficiency indices $n_+ = 1$, $n_- = 0$.
   (c) Show how to construct a symmetric operator with any given pair of deficiency indices.

2. Let A be a closed symmetric operator and suppose that A has a self-adjoint extension. Is it possible for A to have a closed symmetric extension $\tilde{A}$ so that $\tilde{A}$ has no self-adjoint extensions?

3. Let $p(x)$ be a polynomial with real coefficients and let $A = p(i\,d/dx)$ with domain $C_0^\infty(0, \infty)$ in $L^2(0, \infty)$.
   (a) Prove that A is symmetric.
   (b) How are the values of $p(x)$ related to the deficiency indices of A?
   (c) Prove (without using Theorem X.3) that if $p(x)$ has only even powers then the deficiency indices of A are equal.
   (d) Prove that if the degree of p is odd, then the deficiency indices of A are unequal.

†4. Let M and N be closed subspaces of a separable Hilbert space. Prove that if $\dim M > \dim N$, then there exists a $u \in M$, $\|u\| = 1$, so that $u \in N^\perp$.

†5. Complete the analysis of Example 2 of Section X.1 by showing that the self-adjoint extensions of A correspond to the various boundary conditions at zero stated in the example.

6. Classify the self-adjoint extensions of $-d^2/dx^2$ on $C_0^\infty(0, 2\pi)$ and interpret in terms of scattering on a circle with a distinguished point.

7. Prove that if $V(x)$ decreases as $x \downarrow 0$ in $(0, \infty)$, then $-d^2/dx^2 + V(x)$ is limit circle at zero. Hint:
   (a) First show that we may assume $V(x) < 0$ near zero without loss of generality.
   (b) Approximate $V(x)$ near zero by a decreasing step function $\tilde{V}(x)$ (infinitely many steps) so that $|V(x) - \tilde{V}(x)|$ is bounded near zero and show that $-d^2/dx^2 + V(x)$ is limit circle if and only if $-d^2/dx^2 + \tilde{V}(x)$ is limit circle near zero.
   (c) Show that $-d^2/dx^2 + \tilde{V}(x)$ is limit circle by investigating the behavior of the solutions of $\varphi''(x) = \tilde{V}(x)\varphi(x)$ and showing they are both L^2 near zero.

8. Let V be a continuous function on $(0, \infty)$ and suppose that $-d^2/dx^2 + V$ is bounded from below on $C_0^\infty(0, \infty)$.
   (a) Let E be strictly less than the lower bound of $-d^2/dx^2 + V$. Prove that no solution of $-u'' + Vu = Eu$ has more than one zero. Hint: Prove first that any $\psi \in C_0^\infty[a, b]$, $0 < a < b < \infty$, with $\psi(a) = \psi(b) = 0$ obeys
   $$\int_a^b [|\psi'(x)|^2 + V(x)|\psi(x)|^2]\,dx > E\int_a^b |\psi(x)|^2\,dx$$
   (b) Now let $W \geq V$ pointwise. Prove that if $-d^2/dx^2 + V$ is limit point at 0, then so is $-d^2/dx^2 + W$.

   Remarks (1) The above is taken from the article of Kurss quoted in the notes to Section X.1. (2) There is a conjecture of K. Jörgens generalizing this: Let $M \subset \mathbb{R}^n$ be an open set whose complement has measure zero. Let V, W be continuous on M so that $-\Delta + V$ is bounded below and essentially self-adjoint on $C_0^\infty(M)$. If $W \geq V$, then $-\Delta + W$ is also essentially self-adjoint on $C_0^\infty(M)$.

9. Let $\chi(x)$ be a function on $[0, \infty)$ which is C^∞, which vanishes if $x < 1$ and which equals 1 if $x > 2$. Let $\psi \in C_0^\infty(\mathbb{R}^n)$ and let $\psi_m(x) = \psi(x)\chi(m|x|)$. If $n \geq 5$, prove that $\psi_m \xrightarrow{L^2} \psi$, $-\Delta\psi_m \xrightarrow{L^2} -\Delta\psi$, and conclude that $-\Delta$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n/\{0\})$ if $n \geq 5$. (See the last example in the Appendix to Section X.1.)

†10. Prove the estimate (X.17).

11. Construct a potential V on $[0, 1]$ so that $\lim_{r\to 0} V(r) = -\infty$ but with $-d^2/dx^2 + V$ in limit point case at 0 (cf. Problem 7). (Hint: Take V to be piecewise constant with steps of size $-a_n$ where $a_1 a_2^{-1}, a_3 a_2^{-1}, a_3 a_4^{-1}, \ldots, a_{2n-1}a_{2n}^{-1}, a_{2n+1}a_{2n}^{-1}$ are all very small.

†12. Fill in the details of the example of limit point-limit circle behavior for the potentials $V_{ab}(x) = 2x^{-2} - 9x^4(a - 2b\cos(2x^3))$ (see the Notes to Section X.1).

†13. Prove part (b) of Theorem X.13.

14. Let V be a measurable function on $\mathbb{R}^3$ and suppose that $V(r) \to 0$ as $r \to \infty$. If $D(V) \supset D(-\Delta)$, prove that $V \in L^2 + L^\infty$ and thus $< < -\Delta$. (Thus the "potentials" for which one can use Rellich's theorem are precisely the class $L^2 + L^\infty$.)

15. Show that $A = -d^2/dx^2 + V$ is form-bounded from below on $C_0^\infty(0, \infty)$ if $V(x) \geq -1/4x^2$ and is not form-bounded from below if $V(x) \leq c/x^2$ with $c < -\frac{1}{4}$.

16. Let $E > 0$. Prove directly using the kernel for $(-\Delta + E)^{-1}$ that $V(-\Delta + E)^{-1}$ is bounded if $V \in L^2(\mathbb{R}^3)$ and that $\|V(-\Delta + E)^{-1}\| \to 0$ as $E \to \infty$. Conclude from this (without the Sobolev estimate) that $V << -\Delta$.

17. Let V be in the Rollnik class. Prove that:
(a) $\| |V|^{1/2}(-\Delta + E)^{-1}|V|^{1/2} \| \to 0$ as $E \to \infty$
(b) $\| |V|^{1/2}(-\Delta + E)^{-1/2}\| \to 0$ as $E \to \infty$
(c) $\|(-\Delta + E)^{-1/2}|V|(-\Delta + E)^{-1/2}\| \to 0$ as $E \to \infty$
(d) $V \in R$ implies that $V << -\Delta$.

18. Let A and C be essentially self-adjoint on Hilbert spaces $\mathscr{H}_1$ and $\mathscr{H}_2$. Suppose that $B << A$ and that D is C-bounded. Prove that $A \otimes C + B \otimes D$ is essentially self-adjoint on $D(A) \otimes D(C)$.

19. Let A be self-adjoint and let B be symmetric. Suppose that B is A-bounded with relative bound equal to a. Prove that

$$a = \lim_{n \to \infty} \|B(A + in)^{-1}\|$$

20. Let A be self-adjoint. An operator B with $D(B) \supset D(A)$ is called **A-compact** if $B(A - z)^{-1}$ is compact for all $z \in \rho(A)$.
(a) Prove that B is A-compact if $B(A - z)^{-1}$ is compact for one $z \in \rho(A)$.
(b) Suppose that B is symmetric and A-compact. Prove that $B << A$. (Hint: use Problem 19.)

21. Let $\mathscr{H}_m$, $m = \{0, \pm 1, \ldots\}$ be the scale of spaces associated to a positive operator A.
(a) Prove that B is A-compact if and only if B is a compact operator from $\mathscr{H}_{+2}$ to $\mathscr{H}$.
(b) Let β be a symmetric quadratic form which is form bounded with respect to A. Prove that if β defines a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$, then $\beta << A$.
*(c) Let B be a self-adjoint operator which is A-compact. Prove that B defines a compact operator from $\mathscr{H}_{+1}$ to $\mathscr{H}_{-1}$.

22. Use Konrady's trick to prove that $-d^2/dx^2 + p(x)$ is essentially self-adjoint on $C_0^\infty(\mathbb{R})$, where $p(x) = ax^6 + \sum_{i=0}^5 c_i x^i$ and $a > 0$ is sufficiently small.

23. (a) Prove that for any $a > 1$, there is some b, so that for all $\psi \in \mathscr{S}(\mathbb{R})$

$$\|(p^2 + x^2)\psi\|^2 + \|x^4\psi\|^2 \leq a\|(p^2 + x^2 + x^4)\psi\|^2 + b\|\psi\|^2$$

where $p = -i\, d/dx$.
(b) Knowing that $p^2 + x^2 + x^4$ is essentially self-adjoint on $\mathscr{S}(\mathbb{R})$, conclude that it is self-adjoint (in particular, it is closed) on $D(p^2 + x^2) \cap D(x^4)$.
(c) In a similar way prove $D(p^2 + x^2) = D(p^2) \cap D(x^2)$ and conclude that

$$D(p^2 + x^2 + x^4) = D(p^2) \cap D(x^4)$$

24. The purpose of this problem is to prove (without using Theorem X.28) that if $V(x)$ is C^∞, real-valued, and bounded below on $\mathbb{R}^n$, then $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.
(a) Observe that we may assume $V(x) \geq 1$ and prove

$$D((-\Delta + V)^*) = \{\psi \,|\, \psi \in L^2,\ -\Delta\psi + V\psi \in L^2\}$$

where $-\Delta + V$ acts in the sense of distributions.

(b) Explain why every weak solution of $-\Delta\psi + V\psi = 0$ is a C^∞ function.
(c) Show that every weak solution of $\Delta\psi = V\psi$ satisfies

$$\Delta|\psi(x)|^2 \geq |\psi(x)|^2$$

(d) If $\psi \in \mathrm{Ker}((-\Delta + V)^*)$, define $F(r) = \int_{|x|^2 = r} |\psi(x)|^2\, d\Omega$ where $d\Omega$ is the usual measure on the sphere. Show by an integration by parts that F is monotone increasing.
(e) Conclude that $\psi = 0$, so $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$.

25. (Stieltjes moment condition)
(a) Prove that a sequence of real numbers $\{a_n\}_{n=0}^\infty$ are the moments of a measure with support on the positive half line if and only if

$$\sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m} \geq 0 \qquad \text{and} \qquad \sum_{n,m=0}^{N} \bar{\beta}_n \beta_m a_{n+m+1} \geq 0$$

for all N and all $\langle \beta_1, \ldots, \beta_N \rangle \in \mathbb{C}^N$. (Hint: Mimic the proof of the Hamburger moment condition (Section X.1) but use the Friedrichs extension.)
(b) Prove that if in addition to the positivity requirements the a_n satisfy $|a_n| \leq CD^n(2n)!$, then the solution of part (a) is unique. (Hint: Use Theorem X.40.)

26. Construct a semibounded symmetric operator which has a nonsemibounded self-adjoint extension.

27. Let A be a symmetric operator with an invariant domain.
(a) Let B be the Friedrichs extension of $A^2 \upharpoonright D(A)$. Prove that $B = A^*\bar{A}$.
(b) Let $C = \bar{A}A^*$. Prove that C is a self-adjoint extension of $A^2 \upharpoonright D(A)$ and that one has $Q(C) = D(A^*)$.

28. Let A be a symmetric operator and suppose that $D(A^2)$ is dense. Prove that if A^2 is essentially self-adjoint on $D(A^2)$, then A is essentially self-adjoint. (Hint: First prove $(A^*)^2 \subset (A^2)^*$.)

29. Let A be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Prove that $\psi \in \mathscr{H}$ is an analytic vector for A if and only if the function $f(t) = e^{itA}\psi$ is the restriction to the real axis of a function analytic in the strip $|\mathrm{Im}\ t| < b$ for some $b > 0$.

30. The purpose of this problem is to prove von Neumann's theorem (Theorem VIII.14). Let U, V obey the Weyl relations $U(t)V(s) = e^{its}V(s)U(t)$. Let $\alpha > 0$ and let f be of the form $f(s, t) = s^n t^m \exp(-\alpha(s^2 + t^2))$. For $\psi \in \mathscr{H}$, define:

$$W_\psi(f) = \int f(s, t)U(t)V(s)\psi\, ds\, dt$$

(a) Prove that $\{W_\psi(f) \,|\, \psi \in \mathscr{H}\}$ is total in $\mathscr{H}$. Let D be the finite linear span of $\{W_\psi(f)\}$.
(b) Prove that $U(t_0)W_\psi(f) = W_\psi(f(s, t - t_0))$ and that

$$V(s_0)W_\psi(f) = W_\psi(f(s - s_0, t)e^{-its_0})$$

and use this to prove that each W_ψ is an analytic vector for P and for Q.
(c) Prove that $PW_\psi(f) = W_\psi(i\,\partial_t f)$ and that $QW_\psi(f) = W_\psi(i\,\partial_s f) + W_\psi(-tf)$. Use this to prove that D is a set of analytic vectors for $N = \frac{1}{2}(P^2 + Q^2 - 1)$.
(d) Let $A = \frac{1}{2}\sqrt{2}\,(Q + iP)$. Prove that A and A^* are defined on $C^\infty(N)$ and map $C^\infty(N)$ into itself. (Hint: Use the method of Section X.5.) Prove that $N = A^*A$ on vectors in $C^\infty(N)$.

(e) Let $\psi \neq 0$ be in the range of a spectral projection $E_{(n-1,n]}$ for N. Prove that $N^m A\psi = A(N-1)^m\psi$.
(f) Under the conditions in (e), prove that

$$(n-1)(n-2)^m\|\psi\|^2 < (A\psi, N^m A\psi) \leq n(n-1)^m\|\psi\|^2$$

and conclude that $A\psi$ is in the range of the spectral projection $E_{(n-2,n-1]}$ and that $A\psi \neq 0$ if $n \geq 1$.
(g) If ψ obeys the conditions of (e), prove that $A^n\psi = \varphi \neq 0$ but $A\varphi = 0$. Prove that $N\psi = n\psi$ and that $\psi = (1/n!)(A^*)^n\varphi$.
(h) By picking an orthonormal basis for $\{\varphi \mid A\varphi = 0\}$, complete the proof of von Neumann's theorem.

31. Use the ideas of Problem 30 to prove that the Hermite functions are a basis for $L^2(\mathbb{R}, dx)$.

†*32.* Work out the details of all the statements about lower bounds and deficiency indices in Example 1 of Section X.3.

33. (a) Let $A_1, \ldots, A_n$ be an n-tuple of symmetric operators on a dense set $D \subset \mathscr{H}$. Call $\langle A_1, \ldots, A_n\rangle$ closed if D with the norm $|||\psi||| = \sum_{i=1}^n \|A_i\psi\| + \|\psi\|$ is a Banach space. Prove that any such n-tuple has a smallest closed extension.
(b) Let $\langle A_1, \ldots, A_n\rangle$ be an n-tuple of symmetric operators closed in the sense of (a). Prove that $\sum_{i=1}^n A_i^* A_i$ defined on $\{\psi \mid \psi \in D; A_i\psi \in D(A_i^*)\}$ is self-adjoint.
(c) Let $\mathbf{A}(x)$ be an $\mathbb{R}^3$-vector-valued function on $\mathbb{R}^3$ which is locally square integrable and let $V(x)$ be a positive function which is locally L^1. Find a "natural" definition of

$$H = -\frac{1}{2m}\left(\frac{1}{i}\nabla - \frac{e}{c}\mathbf{A}\right)^2 + V$$

†*34.* Let q_n be a counting of the rationals and let a be a quadratic form on $C_0^\infty(\mathbb{R})$ given by

$$a(\psi, \varphi) = \sum_{n=0}^{\infty} 2^{-n}\overline{\psi(q_n)}\varphi(q_n)$$

Let $N = -d^2/dx^2 + 1$ on $L^2(\mathbb{R})$.
(a) Prove that for all $\varphi, \psi \in C_0^\infty(\mathbb{R})$, and some constant D

$$|a(\varphi, \psi)| \leq D\|N^{1/2}\varphi\|\,\|N^{1/2}\psi\|$$

and conclude that there is an operator A on $\mathscr{L}(\mathscr{H}_{+1}, \mathscr{H}_{-1})$ associated to a.
(b) Prove that $\hat{A}$ has $D(\hat{A}) = \{0\}$.

35. Let N be an operator which is self-adjoint with $N \geq 1$. Suppose that a is a symmetric quadratic form with form domain $Q(a) = D(N^2)$ with (i) $\pm a \leq cN^2$; (ii) $\pm i[N, a] \leq dN$ (as forms on $D(N^2)$ where we use (i) to extend a to a form on $D(N)$).
(a) For $\varphi, \psi \in D(N^2)$, prove that

$$a(\varphi, \psi) = a(N^{-1}\varphi, N\psi) - [a, N](N^{-1}\varphi, \psi)$$

and conclude that $|a(\varphi, \psi)| \leq (c+d)\|\varphi\|\,\|N^2\psi\|$.
(b) Prove that there is a symmetric operator A defined on $D(N^2)$ so that AN^{-2} is bounded and $(\varphi, A\psi) = a(\varphi, \psi)$ for all $\varphi, \psi \in D(N^2)$.
(c) For each $\lambda > 0$, define a quadratic form $\delta(\lambda)$ on $\mathscr{H}$ by

$$\delta(\lambda) = \lambda^2(N+\lambda)^{-2}[N, a](N+\lambda)^{-1} + \lambda^2(N+\lambda)^{-1}[N, a](N+\lambda)^{-2}$$

Prove that $\delta(\lambda)$ is an antisymmetric form which is bounded with $\|\delta(\lambda)\| \leq 2d$. Let $\Delta(\lambda)$ denote the skew-symmetric operator associated to δ.
(d) Prove that $\|\Delta(\lambda)N^{-1}\| \to 0$ as $\lambda \to \infty$ and conclude that $\Delta(\lambda) \to 0$ strongly as $\lambda \to \infty$.
(e) By taking matrix elements, prove that for any $\theta \in D(A^*)$,

$$A[\lambda^2(N+\lambda)^{-2}]\theta = [\lambda^2(N+\lambda)^{-2}]A^*\theta + \Delta(\lambda)\theta$$

(f) Let $\theta(\lambda) = \lambda^2(N+\lambda)^{-2}\theta$. Prove that $\theta(\lambda) \to \theta$, $A\theta(\lambda) \to A^*\theta$ and conclude that A is essentially self-adjoint.

Remark The above generalization of the Nelson commutator theorem is a special case of a theorem of Jaffe which allows $\pm a \leq cN^2$ to be replaced by $\pm a \leq cN^m$ for some fixed m; see the paper of McBryan quoted in the Notes to Section X.5.

36. Suppose that each component of $\mathbf{A}$ is a real-valued function in $L^3(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and that V is in $R + L^\infty(\mathbb{R}^3)$ where R is the Rollnik class. For $\varphi, \psi \in Q(\Delta)$, define

$$M(\varphi, \psi) = \left(\frac{1}{i}\nabla\varphi, \mathbf{A}\psi\right) + \left(\mathbf{A}\varphi, \frac{1}{i}\nabla\psi\right) + (\mathbf{A}\varphi, \mathbf{A}\psi)$$

Prove that M is a $-\Delta$ form bounded perturbation with relative bound zero and conclude that there is a unique self-adjoint operator H with $Q(H) = Q(\Delta)$ and

$$(\varphi, H\psi) = (\varphi, -\Delta\psi) + M(\varphi, \psi) + (\varphi, V\psi)$$

37. Extend Theorem X.22 and Problem 36 to the many-body case.

38. Use the methods of Sections X.4 and X.5 to prove that the $L^2(\mathbb{R}^{3N+3})$ operator

$$-(2M_0)^{-1}(\partial_0 - ie\mathbf{A})^2 - (2m)^{-1}\sum_{n=1}^N(\partial_n - ie\mathbf{A})^2 - Ne^2\sum_{n=1}^N|\mathbf{x}_i - \mathbf{x}_0|^{-1}$$
$$+\frac{1}{2}e^2\sum_{n\neq m}|\mathbf{x}_n - \mathbf{x}_m|^{-1} + e\mathbf{E}_0\cdot\left(\mathbf{x}_0 - \sum_{n=1}^N\mathbf{x}_n\right)$$

is essentially self-adjoint on $C_0^\infty(\mathbb{R}^{3N+3})$ if $\mathbf{A} \in C^1(\mathbb{R}^3)_{\text{loc}}$.

†*39.* Show by example that a self-adjoint operator A may have a domain of essential self-adjointness which is disjoint from $D(A^2)$.

40. Let $A = i\,d/dx$ with domain $D(A) = \{\varphi \in L^2[0, 1] \mid \varphi \in AC[0, 1],\ \varphi' \in L^2[0, 1],$ and $\varphi(0) = \varphi(1)\}$. A is self-adjoint. Let $D = \{\varphi \in L^2[0, 1] \mid \varphi$ has an analytic periodic extension to all of $\mathbb{C}$ with x-period one and $\varphi(0) = 0 = \varphi(1)\}$.
(a) Prove that D is a dense set of analytic vectors for A.
(b) Is $A \upharpoonright D$ essentially self-adjoint?

41. Let $U(a, R)$ be a one-dimensional representation of the three-dimensional special Euclidean group. By showing that the spectrum of the momentum must be rotation invariant and using the fact that $SO(3)$ has no nontrivial one-dimensional representations, prove that $U(a, R) = 1$ for all a, R.

†*42.* The purpose of this problem is to prove Theorem X.40.
(a) Let φ be a semianalytic vector for $A \geq 0$. Suppose that $\tilde{A} \geq 0$ is a self-adjoint extension of A_φ on $\mathscr{H}_\varphi$ (for notation see Section X.6). Prove that $\cos(t\tilde{A}^{1/2})$ is

uniquely determined by the numbers $(\psi, A_\varphi^n \psi)$, where $\psi \in D_\varphi$. Conclude that there is at most one positive self-adjoint extension of A_φ.

(b) Prove that there is at most one semibounded extension of A_φ.

(c) Use Theorem X.24 to conclude that A_φ is essentially self-adjoint.

(d) Prove Theorem X.40 by using Nussbaum's lemma.

†43. (a) Prove part (b) of Theorem X.41. (Hint: let $\mathscr{P}_n$ be the polynomials of degree n in $\Phi_S(f)$. Prove by induction that $\mathscr{P}_n\Omega_0$ is dense in $\mathscr{H}_s^{(n)}$).

(b) Prove part (a) (iii) of Theorem X.43.

‡44. Prove that the map $E: \mathscr{S}_{\mathbb{R}}(\mathbb{R}^4) \to L^2(H_m, d\Omega_m)$ defined by $Ef = \sqrt{2\pi}\, \hat{f} \restriction H_m$ has a dense range.

45. Prove that as quadratic forms on $D_{\mathscr{S}} \times D_{\mathscr{S}}$,

$$N = \int_{\mathbb{R}^3} a^\dagger(p)a(p)\, dp$$

$$H_0 \equiv d\Gamma(\mu) = \int_{\mathbb{R}^3} \mu(p)a^\dagger(p)a(p)\, dp$$

†46. Prove (X.76), (X.78), (X.79).

47. Prove that if $g \in L^p(\mathbb{R})$, $1 < p \leq 2$, then $\hat{g}(\sum k_i) \prod_{i=1}^n \mu(k_i)^{-1/2} \in L^2(\mathbb{R}^n)$. (Hint: Use the Hausdorff–Young and Young inequalities.)

48. Let $\mathscr{H}$ be a Hilbert space and $A_1, A_2, \ldots$ a sequence of commuting self-adjoint operators. Suppose that D is a dense domain contained in the domain of each A_i which is invariant under each A_i. Let $\psi_0 \in D$ and define $\circ A_1 \cdots A_n \circ$ recursively by setting $\circ A_1 \cdots A_n \circ = A_1 \cdots A_n + P(A_1, \ldots, A_n)$ where $P(A_1, \ldots, A_n)$ is a polynomial of total degree $n-1$ and individual degree 1, so that

$$((\circ A_1 \cdots A_n \circ)\psi_0, (\circ A_{i_1} \cdots A_{i_m} \circ)\psi_0) = 0$$

for each $\{i_1, \ldots, i_m\} \subsetneq \{1, \ldots, n\}$ and $((\circ A_1 \cdots A_n \circ)\psi_0, \psi_0) = 0$.

(a) Show that $\circ A_1 \cdots A_n \circ$ is uniquely defined for each $n \geq 1$.

(b) If φ is the canonical field on $\mathscr{F}_s(\mathscr{H})$ and $f_n \in \mathscr{H}_C$, and $\psi_0 = \Omega_0$, show that

$$\circ \varphi(f_1) \cdots \varphi(f_n) \circ = :\varphi(f_1) \cdots \varphi(f_n):$$

(c) Show that for each n, the Wick power of the canonical field is the regular power plus a polynomial of lower degree in the regular powers and vice versa.

(d) Show that $:\varphi_m(x, n)^4:$ (introduced in the proof of Theorem X.45) may be written

$$:\varphi_m(x, n)^4: = \varphi_m(x, n)^4 - c_1\varphi_m(x, n)^2 - c_2$$

where c_1 and c_2 depend on n but not on x.

49. Let A be the infinitesimal generator of a contraction semigroup on a Banach space X. Show that for all $\varphi \in X$, $\lim_{n\to\infty} (1 + (t/n)A)^{-n}\varphi = e^{-tA}\varphi$. *Reference*: Kato's book on perturbation theory, pp. 478–480.

50. Let A be an accretive operator on a Hilbert space $\mathscr{H}$.

(a) Show that $J = (I - A)(I + A)^{-1}$ is a (not necessarily everywhere defined) closed contraction operator.

(b) Show that the accretive extensions of A are in one-to-one correspondence with the contraction extensions of J.

(c) Use parts (a) and (b) to prove that a maximal accretive operator on a Hilbert space generates a contraction semigroup.

51. Let $T(t)$ be a strongly continuous semigroup on a Banach space X. Define $\omega_0 = \inf_{t>0} t^{-1} \log\|T(t)\|$.

(a) Prove that $\omega_0 = \lim_{t\to\infty} t^{-1} \log\|T(t)\|$.

(b) Show that for any $\omega_1 > \omega_0$, there is a constant M so that $\|T(t)\| \leq Me^{\omega_1 t}$ for all $t > 0$.

52. Let A be an accretive operator on a Banach space X. Prove that A is closable. (Hint: If A is not closable, there exists a sequence $\varphi_n \in D(A)$ such that $\varphi_n \to 0$ and $A\varphi_n \to \psi$ with $\|\psi\| = 1$. Let $\eta \in D(A)$ with $\|\eta\| = 1$ and $\|\eta - \psi\| > \frac{1}{2}$. Let ℓ_n be a sequence of normalized tangent functionals to the vectors $\eta + c\varphi_n$. Use Alaoglu's theorem to derive a contradiction for appropriate $c > 0$.)

53. Prove that $e^{\Delta t}$ is a continuous L^p-contractive semigroup by using Young's inequality and the explicit form for the kernel.

54. Let $q(x)$ be a bounded, real-valued, continuous function. Prove that $e^{t(\Delta - q)}$ is positivity preserving on $C_\infty(\mathbb{R}^n)$.

55. Fill in the details in the proof of Theorem X.47b.

†56. Prove Theorem X.53 by using the technique of Theorems X.12 and X.50. (Hint: First show that given $\theta_1 < \theta$, one can choose $\omega > 0$ so that $\|B(A - (\lambda - \omega))^{-1}\| \leq \frac{1}{2}$ for all $\lambda \notin \overline{S}_{\pi/2-\theta_1}$.)

57. (a) Prove directly that

$$(e^{z\Delta}f)(x) = (4\pi z)^{-n/2} \int_{\mathbb{R}^n} \exp\left(-\frac{|x-y|^2}{4z}\right) f(y)\, dy$$

is a bounded holomorphic semigroup of angle $\pi/2$ on $C_\infty(\mathbb{R}^n)$.

(b) Prove directly that as an operator on $C_\infty(\mathbb{R}^n)$,

$$\|\partial_i e^{t\Delta}\| \leq Ct^{-1/2}$$

Conclude that $\partial_i(-\Delta + 1)^{-1}$ is bounded on $C_\infty(\mathbb{R}^n)$ so that $D(\Delta) \subset D(\partial_i)$ as operators on $C_\infty(\mathbb{R}^n)$.

†58. Prove Corollary 2 to Theorem X.52.

59. Let $S(s) = e^{-sB}$ and $T(t) = e^{-tA}$ be contraction semigroups on a Banach space X. Suppose that for all $s > 0$ and $t > 0$, $e^{-sB}e^{-tA} = e^{-tA}e^{-sB}$. Then $R(t) = e^{-tB}e^{-tA}$ is a strongly continuous semigroup. Prove that the generator C of $R(t)$ satisfies

$$(I + C)^{-1} = \int_{-\infty}^{\infty} (\tfrac{1}{2} + iy + A)^{-1}(\tfrac{1}{2} - iy + B)^{-1}\, dy$$

60. Let $K_1(\mathbb{R}^3)$ be the closure of $\mathscr{S}(\mathbb{R}^3)$ in the norm $\|\varphi\|_1^2 = \int_{\mathbb{R}^3} |\nabla\varphi|^2\, dx$ and let $\mathscr{H} = K_1(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ with inner product

$$(\langle f_1, f_2\rangle, \langle g_1, g_2\rangle) = \int_{\mathbb{R}^3} (\overline{\nabla f_1} \cdot \nabla g_1 + \overline{f_2}\, g_2)\, dx$$

Let A be the operator $\begin{pmatrix} 0 & I \\ \Delta & 0 \end{pmatrix}$ with domain consisting of all pairs $\langle f_1, f_2 \rangle$ with $f_1, f_2 \in \mathscr{S}(\mathbb{R}^3)$.

(a) Show that iA is symmetric.

(b) Show that iA is essentially self-adjoint by showing that its deficiency indices are $\langle 0, 0 \rangle$.

(c) Show that $D(\overline{(iA)}) = \{\langle f_1, f_2 \rangle \mid \Delta f_1 \in L^2(\mathbb{R}^3), f_2 \in K_1(\mathbb{R}^3)\}$.

(d) Let $U(t) = e^{i(\overline{iA})t} = e^{-\overline{tA}}$ and for $\langle f_1, f_2 \rangle \in D(\overline{A})$ set $\langle u_1(x, t), u_2(x, t) \rangle = U(t)\langle f_1, f_2 \rangle$. Prove that

$$\left(\frac{\partial^2}{\partial t^2} - \Delta\right) u_1(x, t) = 0, \qquad \|u_1(x, t) - f_1(x)\|_{L^2(\mathbb{R}^3)} \to 0$$

and

$$\left\| \frac{\partial}{\partial t} u_1(x, t) - f_2(x) \right\|_{L^2(\mathbb{R}^3)} \to 0 \qquad \text{as} \quad t \to 0$$

61. Let $\{T(t)\}_{t \geq 0}$ be a family of operators on a reflexive Banach space X so that

(i) $T(t + s) = T(t)T(s)$

(ii) $\bigcup_{t>0} \mathrm{Ran}(T(t))$ is dense in X

(iii) $\ell(T(t)\varphi)$ is measurable for each fixed $\varphi \in X$ and $\ell \in X^*$

(iv) $\|T(t)\| \leq 1$ for all t.

Prove that $T(t)$ is strongly continuous. (Hint: Mimic the proof of Theorem VIII.9.)

†*62.* Let $A^\dagger$ and A be the operators defined in Example 2 of Section 6 and let $H_0 = A^\dagger A + \frac{1}{2}$, $V = x^4 = ((A + A^\dagger)/\sqrt{2})^4$.

(a) Prove that

$$\|[H_0^{3/2}, [H_0^{3/2}, V]]\varphi\| \leq e_1 \|H_0^3 \varphi\| + e_2 \|\varphi\|$$

for some constants e_1 and e_2. (Hint: Look at each term in V separately and for each term prove the estimate on the nth Hermite function.)

(b) Use (a) to show that for each $\varepsilon > 0$ there is an M_2 so that (X.109) holds.

(c) Use similar methods to prove (X.110).

63. (a) Prove that the weak topology on the unit ball in a separable Hilbert space is metrizable.

(b) Conclude that the balls in a separable Hilbert space are weakly sequentially complete.

64. Let

$$\tilde{p}(x, y; t) = (4\pi D t)^{-n/2} e^{-|x-y|^2/4Dt}$$

for some D with $\mathrm{Re}\, D \geq 0$, $D \neq 0$. Suppose that there is a *signed* measure μ on the path space Ω of Section X.11 so that $\int \varphi \, d\mu$ is given by the right-hand side of (X.122) but with p replaced by $\tilde{p}$ for $\varphi \in C_{\mathrm{fin}}(\Omega)$. Given $t_1, \ldots, t_n$, let $C^{t_1, \ldots, t_n}$ denote those functions in $C_{\mathrm{fin}}(\Omega)$ of the form $F(\omega(t_1), \ldots, \omega(t_n))$.

(i) If $\mathrm{Re}\, D = 0$, prove that

$$\sup\left\{\left|\int \varphi \, d\mu\right| \,\middle|\, \|\varphi\|_\infty = 1, \varphi \in C^{t_1}(\Omega)\right\} = \infty$$

and conclude that no such signed measure exists.

(ii) If $\mathrm{Re}\, D > 0$, prove that

$$\sup\left\{\left|\int \varphi \, d\mu\right| \,\middle|\, \|\varphi\|_\infty = 1, \varphi \in C^{t_1, \ldots, t_n}(\Omega)\right\} = (|D|/\mathrm{Re}\, D)^n$$

and conclude that no such signed measure exists unless $\mathrm{Im}\, D = 0$.

65. Let Ω_α denote the Hölder continuous paths of order α for some $\alpha < \frac{1}{2}$. Define functions x and x_n from $\Omega \times [0, \infty)$ to $\mathbb{R}$ by

$$x(\omega, t) = \begin{cases} \omega(t) & \text{if} \quad \omega \in \Omega_\alpha \\ 0 & \text{otherwise} \end{cases}$$

and let

$$x_n(\omega, t) = \begin{cases} \omega(m/n) & \text{if } \omega \in \Omega_\alpha \text{ and } m/n \leq t < (m+1)/n \\ 0 & \text{otherwise} \end{cases}$$

(a) Prove that each $x_n(\omega, t)$ is Borel measurable.

(b) Prove that $x_n(\omega, t) \to x(\omega, t)$ pointwise on $\Omega \times [0, \infty)$ as $n \to \infty$ and conclude that $x(\cdot, \cdot)$ is Borel measurable.

(c) Let S have Lebesgue measure zero in $\mathbb{R}^3$. Let $\Omega_S = \{\langle \omega, t \rangle \in \Omega_\alpha \times [0, \infty) \mid \omega(t) \in S\}$. Prove that Ω_S is measurable.

(d) For each $t > 0$, prove that $\mu_x\{\omega \mid \langle \omega, t \rangle \in \Omega_S\} = 0$ and conclude by Fubini's theorem that $(d\mu_x \otimes dt)(\Omega_S) = 0$.

(e) Complete the proof of the lemma following Theorem X.67 by showing that for almost all $\omega \in \Omega$, $\{t \mid \langle \omega, t \rangle \in \Omega_S\}$ has Lebesgue measure zero.

66. Let H_0 be a self-adjoint operator on a Hilbert space $\mathscr{H}$. Let $t \to V(t)$ be a strongly continuous map from $\mathbb{R}$ into the bounded operators on $\mathscr{H}$ satisfying:

(1) For each t, $V(t)$: $D(H_0) \to D(H_0)$ and $[H_0, V(t)]$ is a bounded operator.

(2) $\|[H_0, V(t)]\|$ is locally bounded.

(a) Using the Dyson expansion and the interaction representation prove that if $\psi \in H_0$, then $\varphi_s(t) = e^{-iH_0 t} \tilde{U}(t, s)\psi$ is a strong solution of

$$\frac{d}{dt} \varphi_s(t) = -i(H_0 + V(t))\varphi_s(t), \qquad \varphi_s(s) = \psi$$

(b) Prove the conclusion of (a) by showing that $H_0 + V(t)$ satisfies the hypotheses of Theorem X.70.

67. Let H_0 be the self-adjoint extension of $-d^2/dx^2$ on $L^2[0, \pi]$ corresponding to the boundary conditions $\varphi(0) = 0 = \varphi(\pi)$. Let $V(x, t) = \alpha(t)x$ where $\alpha(t)$ is a positive C^∞ function with support in the interval $[0, t_0]$ satisfying $\int \alpha(t)\, dt = 1$.

(a) Using the method of Example 1 in Section X.12, find upper and lower bounds for the transition probability at t_0 from the first excited state to the ground state.

(b) Why are these estimates valid for all $t > t_0$ also?

†*68.* (a) Prove that the hypotheses on $q(x, t)$ in Example 2 of Section 12 permit the application of Theorem X.70.

(b) Prove that the hypotheses on $t \to V_1(t)$ and $t \to V_2(t)$ in Theorem X.71 permit the application of Theorem X.70.

69. Let $U(t, s)$ be a strongly continuous unitary propagator on a Hilbert space $\mathscr{H}$. Prove that

$$(\tilde{U}(\sigma)f)(t) = U(t, t-\sigma)f(t-\sigma)$$

is a strongly continuous unitary group on $L^2(\mathbb{R}; \mathscr{H})$.

70. Under suitable hypotheses on $V(x, t)$, prove a Feynman–Kac formula in the time-dependent case.

71. Show that if f and g are real-valued, then the components of $W(t)\langle f, g\rangle$ are real-valued for each t where $W(t)$ is the unitary group defined in Section X.13. Use this to show that the solution of (X.138) is real-valued if the initial data are real-valued.

*72. Suppose that the hypotheses of Theorem X.72 hold. Extend J to a map $\tilde{J}$ from $\mathscr{H}$ to $\mathscr{H}$ obeying (H_0) and (H_0^1). Suppose that $\varphi(s)$ is a continuous $\mathscr{H}$-valued function on $[0, t]$ obeying the integral equation (X.143) (with $\tilde{J}$ replacing J). Prove that φ is actually $D(A)$-valued and continuously differentiable and satisfies (X.142) if $\varphi(0) \in D(A)$.

73. Prove all the higher order estimates needed in the proof of Theorem X.76.

74. Show that if every local solution $\varphi(t)$ of (X.142) obeys $\operatorname{Re}\int_0^t (J(\varphi(s)), \varphi(s))\, ds \leq 0$, then the solutions exist globally in t.

75. By using the theorems in Section X.12 prove global existence, uniqueness, smoothness, continuous dependence on the initial data, and finite propagation speed for the equation

$$u_{tt} - \Delta u + m^2 u = -\lambda u^{2n+1}$$
$$u(0, x) = f(x)$$
$$u_t(0, x) = g(x)$$

where $\lambda > 0$, $x \in \mathbb{R}^2$, and $n = 0, 1, 2, \ldots$.

76. In order to handle the mass zero equation in $\mathbb{R}^3$,

$$u_{tt} - \Delta u = -\lambda |u|^2 u, \qquad \lambda > 0$$
$$u(0, x) = f(x)$$
$$u_t(0, x) = g(x)$$

we rewrite it with a linear term added to both sides,

$$u_{tt} - \Delta u + m^2 u = -\lambda |u|^2 u + m^2 u, \qquad m > 0$$

and then formulate the problem as a first-order equation in t as in Section X.13:

$$\varphi'(t) + iA\varphi(t) = J(\varphi(t))$$
$$\varphi(0) = \langle f, g\rangle$$

where $J(\varphi(t)) = J(\langle u(t), v(t)\rangle) = \langle 0, -\lambda|u|^2 u + m^2 u\rangle$.

(a) Show that the estimates of Lemmas 4 and 5 hold for this new J so by Theorem X.72 we get local existence and uniqueness.

(b) Prove that on any interval $[0, T)$ where a solution exists the energy

$$E(t) = \frac{1}{2}\int_{\mathbb{R}^3} (|\nabla u|^2 + |u_t|^2)\, dx + \frac{\lambda}{4}\int |u|^4\, dx$$

is constant.

(c) Prove that on any interval $[0, T)$ where a solution exists, $\|u(t)\|_2 \leq C + t\sqrt{2E}$.

(d) Use parts (b) and (c) to show that if $T < \infty$, then the solution $\varphi(t)$ is norm bounded on $[0, T)$. Thus, by Theorem X.74, global solutions exist.

(e) Check that the proofs of smoothness and propagation speed one go through as in the case of positive mass.

†77. Prove that

$$\int h\{f, g\}\, dx = \int \{h, f\} g\, dx$$

for any $f, g, h \in C_0^1(\mathbb{R}^{6N})$.

†78. Prove the proposition before Theorem X.78.

79. Let $C_{0,\infty}(\mathbb{R})$ denote the continuous functions vanishing at 0 and ∞. Let $D = d/dx$. Prove that D and $-D$ on the natural domain are accretive, but only one of them generates a contraction semigroup.

80. Let A, J, and $\mathscr{H}$ satisfy the hypothesis of Theorem X.74 (except that J is not required to satisfy the hypothesis of part (b) of Theorem X.73). Suppose that for all k, the solutions of (X.143) are a priori bounded uniformly for all $\|\varphi(0)\| \leq k$. Prove that for each $j = 0, 1, \ldots, n$, and each k, there is a monotone increasing (everywhere finite) function $d_{j,k}(\cdot)$ on $(0, \infty)$ so that

$$\|A^j\varphi_1(t) - A^j\varphi_2(t)\| \leq d_{j,k}(|t|)\|\varphi_1(0) - \varphi_2(0)\|$$

for all solutions φ_i of (X.143) with $\|\varphi_i(0)\| \leq k$. Hint: Use the idea of Theorem X.75 and the trick of Lemma 1.

81. Let C be a complex conjugation on a Hilbert space $\mathscr{H}$. Let A be a symmetric operator with $C : D(A) \to D(A)$ and $AC = CA$. An extension B of A is called **real** if $C : D(B) \to D(B)$ and $BC = CB$.

(a) Let $\{\varphi_n\}_{n=1}^N$ be an orthonormal basis for $\mathscr{K}_+$, the deficiency space for A. Define $J : \mathscr{K}_+ \to \mathscr{K}_+$ by $J(\sum a_n\varphi_n) = \sum \bar{a}_n\varphi_n$. If U is a unitary operator from $\mathscr{K}_+$ to $\mathscr{K}_-$, prove that the associated self-adjoint extension A_U is real if and only if $JCU : \mathscr{K}_+ \to \mathscr{K}_+$ has a matrix w.r.t. $\{\varphi_n\}$ which is its own transpose.

(b) Prove that A always has real self-adjoint extensions.

(c) If A has deficiency indices 1, prove that every self-adjoint extension is real. Verify this in the example $-d^2/dx^2$ on $C_0^\infty(0, \infty) \subset L^2(0, \infty)$.

(d) If A has deficiency indices 2 or more, prove that A has self-adjoint extensions which are not real. Verify this in the example $-d^2/dx^2$ on $C_0^\infty(0, 1) \subset L^2(0, 1)$.

READER'S GUIDE

In this chapter, we develop techniques for proving the existence of solutions of the basic dynamical equations in a wide variety of physical situations. We emphasize the applications to quantum mechanics and quantum field theory, and in these cases the existence of dynamics is "equivalent" to proving that the Hamiltonian is self-adjoint. Thus, these techniques are mainly

methods of proving that a given operator is self-adjoint. The following table lists the sections where various physical operators are proven self-adjoint:

	Sections
Atomic Hamiltonians	2
Stark effect Hamiltonians	5, 1 (Appendix) for the one-dimensional case
Zeeman effect Hamiltonians	4
Anharmonic oscillator	2, 4, 6, 9, 10
Quantum field Hamiltonians	7, 9
Quantum field operators	5, 6, 7

It is not necessary for the reader to know all the material in Chapter IX before studying Chapter X. He should, however, know the basic properties of the Fourier transform presented in Sections IX.1 and IX.2 and the properties of the free Hamiltonian discussed in Section IX.7 since this material is used throughout Chapter X without comment. Other theorems about the Fourier transform (for example, the Paley-Wiener theorems and the interpolation theorems) are also used, but the reader can easily refer back to Chapter IX when necessary.

We give a section by section description of Chapter X below; here is a summary. The fundamental properties of self-adjoint operators are discussed in Section VIII.3 and Sections X.1 and X.2. The reader interested in quantum mechanics should know in addition the material in Section VIII.11 and Sections 1 (Appendix), 2, 3, 4, 5, 11, and 12 of Chapter X. The basic discussions of quantum field theory are given in Section IX.8 and Section X.7. The reader interested in quantum field theory should also know the mathematical techniques in Sections 5, 6, 9, 10, and 11 of Chapter X. Self-adjointness techniques can be used to prove the existence and regularity of solutions for certain types of partial differential equations. Such applications appear in Sections 3, 8, 12, and 13 of Chapter X. The Appendix to Section 1 contains applications to ordinary differential equations.

In Section 1 we describe the closed symmetric extensions of symmetric operators by using the theory of deficiency indices. We also prove von Neumann's theorem that a symmetric operator which commutes with a conjugation has self-adjoint extensions. In the Appendix to Section 1 we discuss Weyl's limit point–limit circle criteria and compare the quantum and classical motions on a half-line.

In Section 2 we prove the Kato–Rellich theorem on small perturbations of self-adjoint operators and the KLMN theorem on small form perturbations. The Kato–Rellich theorem is then used to prove the self-adjointness of atomic Hamiltonians.

In Sections 3 and 4 we apply two distinct notions of positivity. In Section 3 we study positive quadratic forms and discuss properties of the Friedrichs extension. In Section 4 we prove a distribution inequality of Kato and use it to show that $-\Delta + V$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^n)$ if V is locally L^2 and bounded below. This technique is then used to prove the self-adjointness of the Zeeman effect Hamiltonian.

In Section 5 we show that if A is dominated by a strictly positive operator N and $[A, N]$ is suitably small, then A is essentially self-adjoint on any core for N. This result is then applied to prove the self-adjointness of the Stark effect Hamiltonian.

In Section 6 we prove Nelson's analytic vector criterion for self-adjointness.

In Section 7 we define the free scalar hermitian Bose field of mass $m > 0$ and prove that it satisfies the Gårding–Wightman axioms. This section should be read in conjunction with Section IX.8. We also introduce Q space and the spatially cut-off Hamiltonian for the $(\varphi^4)_2$ field theory. In the Appendix, we prove that for different m, the free scalar Hermitian field gives rise to inequivalent representations of the canonical commutation relations.

In Section 8 we discuss the natural generalization of many of these self-adjointness techniques to Banach spaces. We characterize the generators of contraction semigroups (the Hille–Yosida and Lumer–Phillips theorems) and introduce holomorphic semigroups. The techniques are used to prove various properties of the solution of the heat equation.

In Section 9 we discuss a special class of semigroups, hypercontractive semigroups, and prove the essential self-adjointness of the spatially cut-off Hamiltonian for the $(\varphi^4)_2$ quantum field theory.

In Section 10 we continue the discussion of graph limit methods for proving self-adjointness begun in Section VIII.7.

In Section 11 we discuss Feynman path integrals, integration on function space, and prove the Feynman–Kac formula.

In Section 12 we prove the existence of solutions of the equation $U'(t) = -A(t)U(t)$ when $A(t)$ is a suitable family of operators on a Banach space. We apply the result to solve the Schrödinger equation with time-dependent potentials and the heat equation with time-dependent sources and sinks.

In Section 13, we prove the existence, smoothness, and finite propagation speed for the nonlinear equation $(\Box^2 + m^2)u = -\lambda u^3$.

In Section 14 we very briefly describe the reformulation of classical mechanics as a Hilbert space problem.

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